

Magnetic Schrödinger operators on armchair nanotubes

Andrey Badanin *

Evgeny Korotyaev †

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Abstract

We consider the Schrödinger operator with a periodic potential on a quasi 1D continuous periodic model of armchair nanotubes in \mathbb{R}^3 in a uniform magnetic field (with amplitude $B \in \mathbb{R}$), which is parallel to the axis of the nanotube. The spectrum of this operator consists of an absolutely continuous part (spectral bands separated by gaps) plus an infinite number of eigenvalues with infinite multiplicity. We describe all eigenfunctions with the same eigenvalue including compactly supported. We describe the spectrum as a function of B . For some specific potentials we prove an existence of gaps independent on the magnetic field. If $B \neq 0$, then there exists an infinite number of gaps G_n with the length $|G_n| \rightarrow \infty$ as $n \rightarrow \infty$, and we determine the asymptotics of the gaps at high energy for fixed B . Moreover, we determine the asymptotics of the gaps G_n as $B \rightarrow 0$ for fixed n .

1 Introduction and main results

We consider the Schrödinger operator $\mathcal{H}_B = (-i\nabla - \mathcal{A})^2 + V_q$ with a periodic potential V_q on the armchair nanotube $\Gamma^N \subset \mathbb{R}^3$, $N \geq 1$ in a uniform magnetic field $\mathcal{B} = B(0, 0, 1) \in \mathbb{R}^3$, $B \in \mathbb{R}$. The corresponding vector potential is given by $\mathcal{A}(x) = \frac{1}{2}[\mathcal{B}, x] = \frac{b}{2}(-x_2, x_1, 0)$, $x = (x_1, x_2, x_3) \in \mathbb{R}^3$. Our model nanotube Γ^N is a union of edges Γ_ω , i.e.,

$$\Gamma^N = \cup_{\omega \in \mathcal{Z}} \Gamma_\omega, \quad \omega = (n, j, k) \in \mathcal{Z} = \mathbb{Z} \times \mathbb{N}_6 \times \mathbb{Z}_N, \quad \mathbb{N}_m = \{1, 2, \dots, m\}, \quad \mathbb{Z}_N = \mathbb{Z}/(N\mathbb{Z}),$$

see Fig. 1, 2. Each edge $\Gamma_\omega = \{x = \mathbf{r}_\omega + t\mathbf{e}_\omega, t \in [0, 1]\}$ is oriented by the vector $\mathbf{e}_\omega \in \mathbb{R}^3$ and has starting point $\mathbf{r}_\omega \in \mathbb{R}^3$. We have the coordinate $x = \mathbf{r}_\omega + t\mathbf{e}_\omega$ and the local coordinate $t \in [0, 1]$ (length preserving). We define $\mathbf{r}_\omega, \mathbf{e}_\omega, \omega = (n, j, k) \in \mathcal{Z}$ by

$$\mathbf{r}_{n,1,k} = 2nh\mathbf{e}_3 + R(c_{2k}, s_{2k}, 0), \quad \mathbf{r}_{n,4,k} = 2nh\mathbf{e}_3 + R(\cos \beta_k, \sin \beta_k, 0), \quad \beta_k = 2\beta + \phi_{2k},$$

$$\mathbf{r}_{n,2,k} = \mathbf{r}_{n,5,k} = (2n+1)h\mathbf{e}_3 + R(\cos \zeta_k, \sin \zeta_k, 0), \quad \zeta_k = \beta - \alpha + \phi_{2k}, \quad \phi_k = \frac{\pi k}{N},$$

*Arkhangelsk State Technical University, e-mail: a.badanin@agtu.ru

†corresponding author, Institut für Mathematik, Humboldt Universität zu Berlin, e-mail: evgeny@math.hu-berlin.de

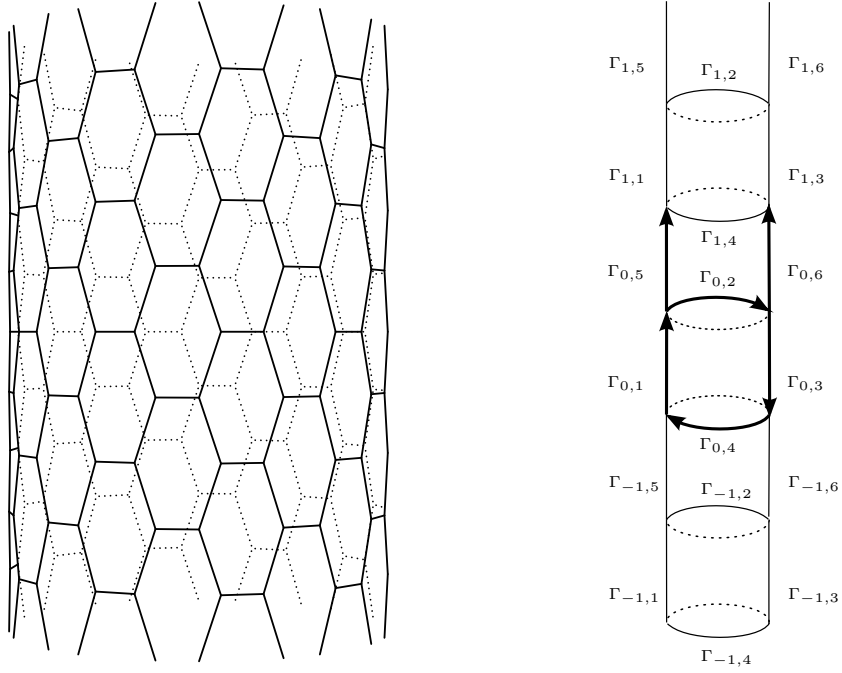


Figure 1: Armchair graph for $N = 10$ and for $N = 1$.

$$\begin{aligned}
\mathbf{r}_{n,3,k} &= \mathbf{r}_{n,6,k} = (2n+1)h\mathbf{e}_3 + R(c_{2k+1}, s_{2k+1}, 0), \\
\mathbf{e}_{n,j,k} &= \mathbf{r}_{n,j+1,k} - \mathbf{r}_{n,j,k}, \quad j = 1, 2, 3, \quad \mathbf{e}_{n,4,k} = \mathbf{r}_{n,1,k+1} - \mathbf{r}_{n,4,k}, \quad \mathbf{e}_{n,5,k} = \mathbf{r}_{n+1,1,k} - \mathbf{r}_{n,5,k}, \\
\mathbf{e}_{n,6,k} &= \mathbf{r}_{n+1,4,k} - \mathbf{r}_{n,6,k}, \quad \sin \beta = \frac{1}{R}, \quad \sin \alpha = \frac{1}{2R}, \quad R = \frac{\sqrt{\cos \phi_1 + \frac{5}{4}}}{\sin \phi_1}, \quad (1.1)
\end{aligned}$$

$0 < \alpha < \beta, \alpha + \beta = \frac{\pi}{N}$ and $h = \sqrt{2 + R_1 R_2 - 2R^2}$, $R_p = \sqrt{(pR)^2 - 1}, p = 1, 2$.

Each edge Γ_ω is the segment and connect the vertices, which lie on the cylinder $\mathcal{C} \equiv \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 = R^2\}$. Note that each edge Γ_ω (without the endpoints) lies inside the cylinder \mathcal{C} . The points $\mathbf{r}_{0,j,k}$ are vertices of the regular N -gon $\mathcal{P}_j, j = 1, 2, 3, 4$. \mathcal{P}_3 (\mathcal{P}_2) arises from \mathcal{P}_1 (\mathcal{P}_4) by the following motion: rotate around the axis of the cylinder \mathcal{C} by the angle $\frac{\pi}{N}$ and translate by $h\mathbf{e}_3$. Repeating this procedure we obtain Γ^N .

For each function y on Γ^N we define a function $y_\omega = y|_{\Gamma_\omega}, \omega \in \mathcal{Z}$. We identify each function y_ω on Γ_ω with a function on $[0, 1]$ by using the local coordinate $t \in [0, 1]$. Define the Hilbert space $L^2(\Gamma^N) = \oplus_{\omega \in \mathcal{Z}} L^2(\Gamma_\omega)$. Our operator \mathcal{H}_B on Γ^N acts in the Hilbert space $L^2(\Gamma^N) = \oplus_{\omega} L^2(\Gamma_\omega)$ and is given by

$$(\mathcal{H}_B f)_\omega = -\partial_\omega^2 f_\omega(t) + q(t)f_\omega(t), \quad \partial_\omega = \frac{d}{dt} - ia_\omega, \quad a_\omega(t) = (\mathcal{A}(\mathbf{r}_\omega + t\mathbf{e}_\omega), \mathbf{e}_\omega), \quad (1.2)$$

see [SDD], where $(V_q f)_\omega = q f_\omega, q \in L^2(0, 1)$ and $\oplus_\omega f_\omega, \oplus_\omega f''_\omega \in L^2(\Gamma^N)$ satisfies

Magnetic Kirchhoff Boundary Conditions: y is continuous on Γ^N and

$$\partial_{\omega_2} y_{\omega_2}(0) - \partial_{\omega_1} y_{\omega_1}(1) + \partial_{\omega_5} y_{\omega_5}(0) = 0, \quad \partial_{\omega_3} y_{\omega_3}(0) - \partial_{\omega_2} y_{\omega_2}(1) + \partial_{\omega_6} y_{\omega_6}(0) = 0,$$

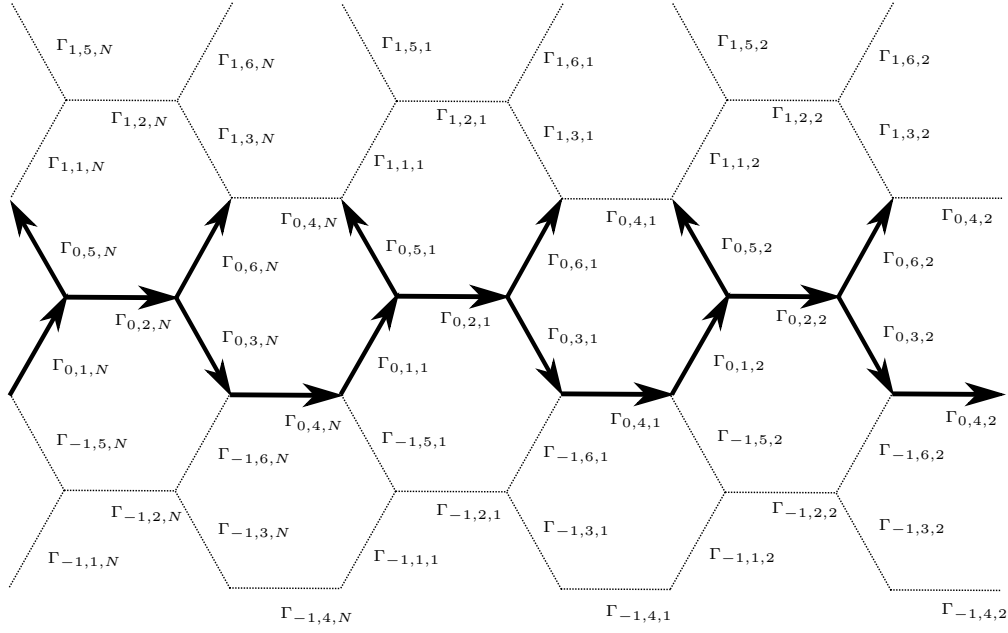


Figure 2: A piece of a nanotube Γ^N . The fundamental domain is marked by a bold line.

$$-\partial_{\omega_3} y_{\omega_3}(1) + \partial_{\omega_4} y_{\omega_4}(0) - \partial y_{n-1,6,k}(1) = 0, \quad -\partial_{\omega_4} y_{\omega_4}(1) + \partial y_{n,1,k+1}(0) - \partial y_{n-1,5,k+1}(1) = 0, \quad (1.3)$$

for all $\omega_j = (n, j, k)$, $(n, j, k) \in \mathbb{Z} \times \mathbb{N}_6 \times \mathbb{Z}_N$.

Condition (1) means that the sum of derivatives of y at each vertex of Γ^N equals 0 and the orientation of edges gives the sign \pm . Such models were introduced by Pauling [Pa] in 1936 to simulate aromatic molecules. They were described in more detail by Ruedenberg and Scherr [RS] in 1953. Further progress had been made toward periodic systems by Coulson in [Co] where a network model of graphite layer was worked out. A network model of a crystal with non-trivial potentials along bonds was studied by Montroll [Mo]. Carbon and boron nitride nanostructures, in particular nanotubes, graphene layers have been modelled by quantum networks with a honeycomb lattice structure in [ALM], [ALM1]. As it is shown in [Ha], Ch.7.3.3, the structure of carbon-boron-nitride single wall nanotubes may be complicated. The edge potential q is not even for such tubes. We consider one of nanotube models, where the potential is not even. The other models can be considered by the similar way.

The standard arguments (see [KL]) yield that \mathcal{H}_B is self-adjoint. For simplicity we shall denote $\Gamma_{\alpha,1} \subset \Gamma^1$ by Γ_α , for $\alpha = (n, j) \in \mathcal{Z}_1 = \mathbb{Z} \times \mathbb{N}_6$. Thus $\Gamma^1 = \cup_{\alpha \in \mathcal{Z}_1} \Gamma_\alpha$, see Fig 1. In Theorem 1.1 we will show that \mathcal{H}_B is unitarily equivalent to $H^a = \oplus_1^N H_k^a$, where the operator H_k^a acts in the Hilbert space $L^2(\Gamma^1)$ and is given by $(H_k^a f)_\alpha = -f''_\alpha + q f_\alpha$, $(f_\alpha)_{\alpha \in \mathcal{Z}_1}$, $(f''_\alpha)_{\alpha \in \mathcal{Z}_1} \in L^2(\Gamma^1)$, and the components f_α satisfy:

$$\begin{aligned} e^{ia_1} f_{n,1}(1) &= f_{n,2}(0) = f_{n,5}(0), & e^{ia_2} f_{n,2}(1) &= f_{n,3}(0) = f_{n,6}(0), \\ e^{ia_1} f_{n,3}(1) &= f_{n,4}(0) = e^{ia_1} f_{n-1,6}(1), & e^{ia_2} s^k f_{n,4}(1) &= f_{n,1}(0) = e^{-ia_1} f_{n-1,5}(1), \end{aligned} \quad (1.4)$$

$$\begin{aligned}
e^{ia_1} f'_{n,1}(1) - f'_{n,2}(0) - f'_{n,5}(0) &= 0, & e^{ia_2} f'_{n,2}(1) - f'_{n,3}(0) - f'_{n,6}(0) &= 0, \\
e^{ia_1} f'_{n,3}(1) - f'_{n,4}(0) + e^{ia_1} f'_{n-1,6}(1) &= 0, & e^{ia_2} s^k f'_{n,4}(1) - f'_{n,1}(0) + e^{-ia_1} f'_{n-1,5}(1) &= 0,
\end{aligned} \quad (1.5)$$

where

$$s = e^{\frac{2\pi i}{N}}, \quad a_1 = \frac{B(R_2 - R_1)}{4}, \quad a_2 = \frac{BR_2}{4}, \quad a = a_1 + a_2 = \frac{B(2R_2 - R_1)}{4}, \quad (1.6)$$

R is given by (1.1), and $R_p = \sqrt{(pR)^2 - 1}$, $p = 1, 2$. For the operator H_k^a we define fundamental solutions $\vartheta_k^{(\nu)} = (\vartheta_{k,\alpha}^{(\nu)})_{\alpha \in \mathbb{Z}_1}$, $\varphi_k^{(\nu)} = (\varphi_{k,\alpha}^{(\nu)})_{\alpha \in \mathbb{Z}_1}$, $\nu = 1, 2$ which satisfy

$$\begin{aligned}
-\Delta y + V_q y &= \lambda y, \quad \text{on } \Gamma^1, & \text{b. c. (1.4), (1.5)} \\
\Theta_{k,0}(1, \lambda) &= \Phi'_{k,0}(1, \lambda) = I_2, & \Theta'_{k,0}(1, \lambda) = \Phi_{k,0}(1, \lambda) = 0,
\end{aligned} \quad (1.7)$$

where $I_n, n \geq 2$ is the $n \times n$ identity matrix and

$$\Theta_{k,n} = \begin{pmatrix} \vartheta_{k,n,5}^{(1)} & \vartheta_{k,n,5}^{(2)} \\ \vartheta_{k,n,6}^{(1)} & \vartheta_{k,n,6}^{(2)} \end{pmatrix}, \quad \Phi_{k,n} = \begin{pmatrix} \varphi_{k,n,5}^{(1)} & \varphi_{k,n,5}^{(2)} \\ \varphi_{k,n,6}^{(1)} & \varphi_{k,n,6}^{(2)} \end{pmatrix}. \quad (1.8)$$

We define the monodromy matrix by

$$\mathcal{M}_k(\lambda) = \begin{pmatrix} \Theta_{k,1} & \Phi_{k,1} \\ \Theta'_{k,1} & \Phi'_{k,1} \end{pmatrix} (1, \lambda). \quad (1.9)$$

This matrix is determined by the fundamental solutions on a fundamental cell $\Gamma_0^1 = \cup_{j=1}^6 \Gamma_{0,j}$. In order to analyse the operator H^a we use the methods based on a research of the monodromy matrix \mathcal{M}_k (see [KL], [KL1], [BBKL], [BBK1], and also [BBK], [CK], [K]).

Let $\sigma_D = \{\mu_n, n \geq 1\}$ be the spectrum of the problem $-y'' + qy = \lambda y, y(0) = y(1) = 0$ (the Dirichlet spectrum). We formulate our first result.

Theorem 1.1. (i) The operator \mathcal{H}_B is unitarily equivalent to $H^a = \oplus_1^N H_k^a$.

(ii) Let $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$. Then for any $\lambda \in \mathbb{C} \setminus \sigma_D$ there exist unique fundamental solutions $\vartheta_k^{(\nu)} = (\vartheta_{k,\alpha}^{(\nu)})_{\alpha \in \mathbb{Z}_1}$, $\varphi_k^{(\nu)} = (\varphi_{k,\alpha}^{(\nu)})_{\alpha \in \mathbb{Z}_1}$, $\nu = 1, 2$. Moreover, each of the functions $\vartheta_{k,\alpha}^{(\nu)}(x, \lambda)$, $\varphi_{k,\alpha}^{(\nu)}(x, \lambda)$, $x \in \Gamma^1$ is analytic in $\lambda \in \mathbb{C} \setminus \sigma_D$ and the monodromy matrix $\mathcal{M}_k(\lambda)$, $\lambda \notin \sigma_D$ has eigenvalues of the form $\tau_{k,1}^{\pm 1}, \tau_{k,2}^{\pm 1}$ and satisfies

$$\det \mathcal{M}_k = 1, \quad \mathcal{M}_k(\lambda)^\top J \mathcal{M}_k(\lambda) = J, \quad \text{where } J = \begin{pmatrix} 0 & \mathbf{j} \\ -\mathbf{j} & 0 \end{pmatrix}, \quad \mathbf{j} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (1.10)$$

Furthermore, the matrix-valued function $\mathcal{R} \mathcal{M}_k \mathcal{R}^{-1}$ is entire, where $\mathcal{R} = I_2 \oplus \varphi_1 I_2$.

For all $B \in \mathbb{R}$ the monodromy matrix \mathcal{M}_k has a simple pole at each point $\lambda \in \sigma_D$, which is an eigenvalue of H_k^a (see Theorem 2.2) and has no any other singularities. Moreover, these poles are independent on the magnetic field. This result is in contrast with the corresponding result for the zigzag tube (see [KL], [KL1]). For the zigzag tube there exist some singular

values of the magnetic field, where the monodromy matrix is not well defined. Moreover, the spectrum is pure point for such singular values and the spectral bands shrink to the points as the magnetic field approach to the singular value.

For the equation $-y'' + q(t)y = \lambda y$ on the real line we introduce the fundamental solutions $\vartheta(t, \lambda)$ and $\varphi(t, \lambda)$, $(t, \lambda) \in \mathbb{R} \times \mathbb{C}$ satisfying $\vartheta(0, \lambda) = \varphi'(0, \lambda) = 1$, $\vartheta'(0, \lambda) = \varphi(0, \lambda) = 0$. We define the functions F, F_- by

$$F = \frac{\varphi'_1 + \vartheta_1}{2}, \quad F_- = \frac{\varphi'_1 - \vartheta_1}{2}, \quad (1.11)$$

where $\varphi_1 = \varphi(1, \cdot)$, $\vartheta_1 = \vartheta(1, \cdot)$, $\varphi'_1 = \varphi'(1, \cdot)$, $\vartheta'_1 = \vartheta'(1, \cdot)$. We formulate the results about the Lyapunov function and the spectrum of H_k^a .

Theorem 1.2. *Let $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$ and let $\tau_{k,1}^{\pm 1}, \tau_{k,2}^{\pm 1}$ be eigenvalues of \mathcal{M}_k . Then*

(i) The Lyapunov functions $F_{k,\nu} = \frac{1}{2}(\tau_{k,\nu} + \tau_{k,\nu}^{-1})$, $\nu = 1, 2$ are branches of $F_k = \xi_k + \sqrt{\rho_k}$ on the two sheeted Riemann surface \mathfrak{R}_k defined by $\sqrt{\rho_k}$ and satisfy:

$$F_{k,\nu} = \xi_k - (-1)^\nu \sqrt{\rho_k}, \quad \xi_k = \frac{9F^2 - F_-^2 - 1}{2} - s_k^2, \quad \rho_k = (9F^2 - s_k^2)c_k^2 + s_k^2 F_-^2, \quad (1.12)$$

$$\det(\mathcal{M}_k - \tau I_4) = (\tau^2 - 2F_{k,1}\tau + 1)(\tau^2 - 2F_{k,2}\tau + 1), \quad (1.13)$$

where

$$c_k = \cos\left(\frac{\pi k}{N} + a\right), \quad s_k = \sin\left(\frac{\pi k}{N} + a\right), \quad (1.14)$$

a is given by (1.6).

(ii) If $F_k(\lambda) \in (-1, 1)$ for some $\lambda \in \mathbb{R}$ and λ is not a branch point of $F_k(\lambda)$, then $F'_k(\lambda) \neq 0$.

(iii) The following identities hold:

$$\begin{aligned} \sigma(H_k^a) &= \sigma_{pp}(H_k^a) \cup \sigma_{ac}(H_k^a), \quad \sigma_{pp}(H_k^a) = \sigma_D, \\ \sigma_{ac}(H_k^a) &= \{\lambda \in \mathbb{R} : F_{k,\nu}(\lambda) \in [-1, 1] \text{ for some } \nu \in \mathbb{N}_2\}, \end{aligned} \quad (1.15)$$

$$\sigma(H_k^{-a}) = \sigma(H_{N-k}^a), \quad \sigma(H_k^{a+\frac{\pi}{N}}) = \sigma(H_{k+1}^a), \quad \sigma(H_k^{a+\pi}) = \sigma(H_k^a) \quad (1.16)$$

(each point of the spectrum is counted with multiplicities). Each point $\lambda_0 \in \sigma_{pp}(H_k^a)$ has an infinite multiplicity.

Remark. 1) We take the branch of $\sqrt{\rho_k}$ such that if $\rho_k(\lambda) > 0, \lambda \in \mathbb{R}$, then $\sqrt{\rho_k(\lambda)} > 0$ and $F_{k,1} = \xi_k + \sqrt{\rho_k} > F_{k,2} = \xi_k - \sqrt{\rho_k}$. Then $\sqrt{\rho_k}$ is not an entire function even for $c_k = 0$ or $s_k = 0$. Using other branches we could define a new function $\sqrt{\rho_k}$ which is entire for $c_k = 0$ or $s_k = 0$, but this choice is not convenient for labeling of endpoints of gaps (see below Theorems 1.3-1.6).

2) The statement (ii) is similar to the standard result of Lyapunov for the Hamilton systems. The similar results hold for the zigzag tube in magnetic field (see [KL],[KL1]).

3) Periodicity of the spectrum with respect to B holds for the zigzag nanotube (see [KL1]).

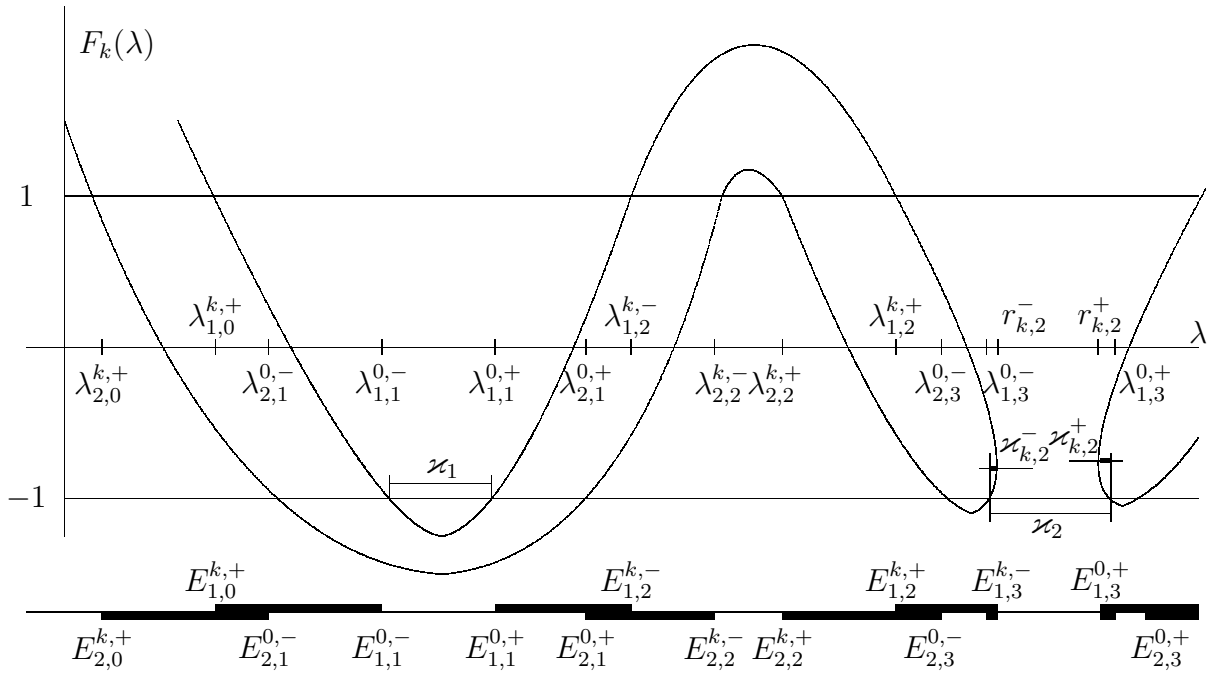


Figure 3: Graph of the function $F_k(\lambda)$ and the spectrum of H_k

4) Below we will sometimes write $c_k(a), F_{k,\nu}(\lambda, a), \dots$ instead of $c_k, F_{k,\nu}(\lambda), \dots$, when several magnetic fields are being dealt with. In order to prove (1.16) we use the identities

$$s_k(-a) = s_{N-k}(a), \quad c_k(-a) = c_{N-k}(a), \quad s_k(a + \frac{\pi}{N}) = s_{k+1}(a), \quad c_k(a + \frac{\pi}{N}) = c_{k+1}(a). \quad (1.17)$$

5) We say that $\{\lambda_0\} \subset \sigma_{pp}(H_k^a)$ is a flat band. The corresponding eigenfunctions of H_k^a have compact supports (shown by Fig.4) and are described in Theorem 2.2.

We define the entire functions

$$D_k^\pm = \det(\mathcal{M}_k \mp I_4) = 4(F_{k,1} \mp 1)(F_{k,2} \mp 1). \quad (1.18)$$

The zeros $\lambda_{\nu,2n}^{k,\pm}, n \geq 0, \nu = 1, 2$, of the function D_k^+ are the periodic eigenvalues. The zeros $\lambda_{\nu,2n-1}^{k,\pm}, (\nu, n) \in \mathbb{N}_2 \times \mathbb{N}$, of D_k^- are the antiperiodic eigenvalues. Let

$$\lambda_{2,0}^{k,+} \leq \lambda_{1,0}^{k,+} \leq \lambda_{1,2}^{k,-} \leq \lambda_{2,2}^{k,-} \leq \lambda_{2,2}^{k,+} \leq \lambda_{1,2}^{k,+} \leq \lambda_{1,4}^{k,-} \leq \lambda_{2,4}^{k,-} \leq \lambda_{2,4}^{k,+} \leq \lambda_{1,4}^{k,+} \leq \dots$$

and

$$\lambda_{2,1}^{k,-} \leq \lambda_{1,1}^{k,-} \leq \lambda_{1,1}^{k,+} \leq \lambda_{2,1}^{k,+} \leq \lambda_{2,3}^{k,-} \leq \lambda_{1,3}^{k,-} \leq \lambda_{1,3}^{k,+} \leq \lambda_{2,3}^{k,+} \leq \dots$$

counted with multiplicities. Such labeling was introduced in [BBK1] for the case $a = 0$, and is associated with the Lyapunov functions $F_{k,1}, F_{k,2}$ (see Fig.3).

A zero of $\rho_k, k \in \mathbb{Z}_N$ is called a **resonance** of H_k^a . There exist real and non-real resonances (see example from [BBKL]). Roughly speaking the simple real resonances create gaps. Note that in the case of zigzag nanotubes all resonances are real (see [KL], [KL1]).

We define the functions

$$u_k(\lambda) = |F_-(\lambda)| - s_k^2, \quad v_k(\lambda) = |F_-(\lambda)| - c_k^2, \quad \lambda \in \mathbb{R}, \quad k \in \mathbb{Z}_N. \quad (1.19)$$

Theorem 1.3. *Let $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$. Then the identity*

$$\sigma_{ac}(H_k^a) = \cup_{(\nu, n) \in \mathbb{N}_2 \times \mathbb{N}} S_{\nu, n}^{k, a}, \quad S_{\nu, n}^{k, a} = [E_{\nu, n-1}^{k, +}, E_{\nu, n}^{k, -}] \quad (1.20)$$

holds, where each spectral band $S_{\nu, n}^{k, a}$ satisfies:

$$E_{\nu, p-1}^{k, \pm} = \lambda_{\nu, p-1}^{k, \pm}, \quad E_{2, p}^{k, \pm} = \lambda_{2, p}^{0, \pm}, \quad E_{1, p}^{k, \pm} = \begin{cases} \lambda_{1, p}^{0, \pm} & \text{if } v_k(\lambda_{1, p}^{0, \pm}) \geq 0 \\ r_{k, n}^{\pm} & \text{if } v_k(\lambda_{1, p}^{0, \pm}) < 0 \end{cases}, \quad p = 2n - 1, \quad (1.21)$$

$$\lambda_{\nu, p}^{k, \pm}(a) = \lambda_{\nu, p}^{0, \pm}(0), \quad E_{2, p}^{k, \pm}(a) = E_{2, p}^{0, \pm}(0), \quad \varkappa_n(a) = \varkappa_n(0), \quad (1.22)$$

where

$$r_{k, n}^- = \min\{\lambda \in \overline{\varkappa}_n : \rho_k(\lambda) = 0\}, \quad r_{k, n}^+ = \max\{\lambda \in \overline{\varkappa}_n : \rho_k(\lambda) = 0\}, \quad \varkappa_n = (\lambda_{1, p}^{0, -}, \lambda_{1, p}^{0, +}). \quad (1.23)$$

Remark. 1) For some specific potentials and some $n \geq 1$ the intervals \varkappa_n are antiperiodic gaps (see below Proposition 3.5 and Theorem 1.6 (i)). These gaps are independent on the magnetic field.

2) We describe $\sigma_{ac}(H_k^a)$ in details in Theorems 3.4, 3.6.

Recall the needed properties of the Hill operator $\tilde{H}y = -y'' + q(t)y$ on the real line with a periodic potential $q(t+1) = q(t), t \in \mathbb{R}$. The spectrum of \tilde{H} is purely absolutely continuous and consists of intervals $[\tilde{\lambda}_{n-1}^+, \tilde{\lambda}_n^-], n \geq 1$. These intervals are separated by the gaps $\tilde{\gamma}_n = (\tilde{\lambda}_n^-, \tilde{\lambda}_{n+1}^+)$ of length $|\tilde{\gamma}_n| \geq 0$. If a gap $\tilde{\gamma}_n$ is degenerate, i.e. $|\tilde{\gamma}_n| = 0$, then the corresponding segments merge. The sequence $\tilde{\lambda}_0^+ < \tilde{\lambda}_1^- \leq \tilde{\lambda}_1^+ < \dots$ is the spectrum of the equation $-y'' + qy = \lambda y$ with 2-periodic boundary conditions, that is $y(t+2) = y(t), t \in \mathbb{R}$. Here equality $\tilde{\lambda}_n^- = \tilde{\lambda}_{n+1}^+$ means that $\tilde{\lambda}_n^\pm$ is an eigenvalue of multiplicity 2. It is well-known that $\mu_n \in [\tilde{\lambda}_n^-, \tilde{\lambda}_{n+1}^+], n \geq 1$. The function F has only simple zeros $\eta_n, n \geq 1$, which satisfy $\eta_1 < \eta_2 < \dots$. We describe the spectral gaps of H_k^a .

Theorem 1.4. *Let $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$. Then*

(i) $\sigma_{ac}(H_k^a) = \mathbb{R} \setminus \cup_{n \geq 0} G_{k, n}^a$, where the gaps $G_{k, n}^a$ satisfy:

$$\begin{aligned} \tilde{\gamma}_0 \subset G_{k, 0}^a &= (-\infty, E_{2, 0}^{k, +}), \quad \tilde{\gamma}_n \subset G_{k, 4n}^a = (E_{2, 2n}^{k, -}, E_{2, 2n}^{k, +}), \quad G_{k, 4n-2}^a = (E_{1, 2n-1}^{k, -}, E_{1, 2n-1}^{k, +}) \subset \varkappa_n, \\ G_{k, 4n-3}^a &= (E_{2, 2n-1}^{k, -}, E_{1, 2n-2}^{k, +}), \quad G_{k, 4n-1}^a = (E_{1, 2n}^{k, -}, E_{2, 2n-1}^{k, +}), \quad \eta_n \in [E_{1, 2n-1}^{k, -}, E_{1, 2n-1}^{k, +}]. \end{aligned} \quad (1.24)$$

If $s_k^2(a) < s_\ell^2(a_1)$ for some $(a_1, \ell) \in \mathbb{R} \times \mathbb{Z}_N$, then

$$G_{k, 4n}^a \subset G_{\ell, 4n}^{a_1}, \quad G_{\ell, 2n-1}^{a_1} \subset G_{k, 2n-1}^a \quad \text{all } n \geq 1. \quad (1.25)$$

Moreover, for all $n \geq n_0$ and some $n_0 \geq 1$

$$G_{k, 4n-2}^a = \begin{cases} \emptyset, & \text{if } (a, k) = (0, 0) \\ \neq \emptyset, & \text{if } (a, k) \neq (0, 0) \end{cases}, \quad G_{k, 2n-1}^a = \emptyset, \quad \text{if } (a, k) \neq (0, 0). \quad (1.26)$$

(ii) If $v_k = |F_-(\lambda)| - c_k^2 \geq 0$ on \varkappa_n for some $n \geq 1$, then $G_{k, 4n-2}^a = \varkappa_n$.

We formulate our main result about the spectrum of H^a .

Theorem 1.5. *Let $a \in [0, \frac{\pi}{2N}]$. Then the following identities hold true:*

$$\sigma(H^a) = \sigma_{pp}(H^a) \cup \sigma_{ac}(H^a), \quad \sigma_{pp}(H^a) = \sigma_D, \quad \sigma(H^a) = \sigma(H^{-a}) = \sigma(H^{a+\frac{\pi}{N}}) \quad (1.27)$$

(each point of the spectrum is counted with multiplicities).

(i) $\sigma_{ac}(H^a) = \mathbb{R} \setminus \cup_{n \geq 0} G_n^a$, where the gaps $G_n^a = \cap_{k \in \mathbb{Z}_N} G_{k,n}^a = (E_n^-, E_n^+)$ satisfy:

$$\tilde{\gamma}_n \subset G_{4n}^a, \quad G_{4n-2}^a \subset \varkappa_n, \quad \eta_n \in [E_{4n-2}^-, E_{4n-2}^+], \quad (1.28)$$

$$G_{4n}^a \subset G_{4n}^{a_1}, \quad G_{2n-1}^{a_1} \subset G_{2n-1}^a, \quad 0 \leq a < a_1 \leq \frac{\pi}{2N}. \quad (1.29)$$

Moreover, for all $n \geq n_0$ and some $n_0 \geq 1$

$$G_{4n-2}^a = \begin{cases} \emptyset, & \text{if } a = 0 \\ \neq \emptyset, & \text{if } a \neq 0 \end{cases}, \quad G_{2n-1}^a = \emptyset, \text{ if } (a, N) \neq (0, 1). \quad (1.30)$$

(ii) The spectrum $\sigma(H^a)$, $a \in (0, \frac{\pi}{2N})$, has an infinite number of gaps $G_{2n}^a \neq \emptyset$ and $|G_{2n}^a| \rightarrow \infty$ as $n \rightarrow \infty$. Moreover, the following asymptotics hold true:

$$E_{4n-2m}^\pm(a) = \left(\pi(n - \frac{m}{2}) \pm \tilde{\theta}_m \right)^2 + q_0 + O(n^{-1}), \quad n \rightarrow \infty, \quad m = 0, 1, \quad (1.31)$$

where $q_0 = \int_0^1 q(t)dt$, $\tilde{\theta}_0 = \arccos(\frac{1}{3}\sqrt{5+4|\cos a|})$, $\tilde{\theta}_1 = \arcsin(\frac{1}{3}\sin a)$. Furthermore, if $N \geq 2$, then all other gaps with sufficiently large energy are empty.

(iii) If $|F_-| \geq \cos^2 a$ on \varkappa_n for some $n \geq 1$, then $G_{4n-2}^a = \varkappa_n$.

Remark. 1) Identities (1.27) show that for analysis of operator H^a , $a \in \mathbb{R}$ it is sufficiently to study $a \in [0, \frac{\pi}{2N}]$.

2) Using the statement (iii) we prove in Proposition 3.5 that each $G_{4n-2}^a = G_{4n-2}^0 \neq \emptyset$, $(a, n) \in \mathbb{R} \times \mathbb{N}_{n_0}$ for any $n_0 \geq 1$ and some non-even potential (which depends on n_0). Note that if the potential is even, then all the gaps G_{4n-2}^a depend on the magnetic field (see below (1.35)).

Recall the definition of the effective masses for the Hill operator. The identity $F(\lambda) = \cos k(\lambda)$, $\lambda \in \mathbb{C}_+$ defines the quasimomentum $k(\lambda)$, which is an analytic function on $\lambda \in \mathbb{C}_+$. With each endpoint of the gap $\tilde{\gamma}_n \neq \emptyset$, we associate the effective mass M_0^+ , M_n^\pm by (we take some branches k such that $k(\lambda) \rightarrow \pi n$ as $\lambda \rightarrow \tilde{\lambda}_n^\pm$)

$$\lambda = \tilde{\lambda}_n^\pm + \frac{(k(\lambda) - \pi n)^2}{2M_n^\pm}(1 + o(1)) \quad \text{as} \quad \lambda \rightarrow \tilde{\lambda}_n^\pm. \quad (1.32)$$

(see [KK]). We formulate results for even potentials. Let $L_{even}^2(0, 1) = \{q \in L^2(0, 1) : q(1-t) = q(t), t \in (0, 1)\}$.

Theorem 1.6. Let $q \in L_{\text{even}}^2(0, 1)$, $(a, n) \in [0, \frac{\pi}{2N}] \times \mathbb{N}$. Then

(i) If $c_k = 0$, then $\rho_k = 0$ and $G_{k,4n-2}^a = \varnothing$. If $c_k \neq 0$, then all resonances are real and $G_{k,4n-2}^a = (r_{k,n}^-, r_{k,n}^+)$. For each $k \in \mathbb{Z}_N$ the gaps $G_{k,4n-2}^a$ satisfy:

$$G_{k,4n-2}^a = \begin{cases} \emptyset, & \text{if } (a, k) = (0, 0) \\ \neq \emptyset, & \text{if } (a, k) \neq (0, 0) \end{cases}, \quad G_{k,2n-1}^a = \emptyset. \quad (1.33)$$

If $s_k^2(a) < s_\ell^2(a_1)$ for some $(a_1, \ell) \in \mathbb{R} \times \mathbb{Z}_N$, then $G_{k,4n-2}^a \subset G_{\ell,4n-2}^{a_1}$.

(ii) The gaps of H^a satisfy

$$G_{4n-2}^a \subset G_{4n-2}^{a_1}, \quad 0 \leq a < a_1 \leq \frac{\pi}{2N}, \quad (1.34)$$

$$G_{4n}^0 = \tilde{\gamma}_n, \quad G_{4n-2}^a = \begin{cases} \emptyset, & \text{if } a = 0 \\ \neq \emptyset, & \text{if } a \neq 0 \end{cases}, \quad G_{2n-1}^a = \emptyset. \quad (1.35)$$

Moreover, if $a \in (0, \frac{\pi}{2N}]$, then $G_{2n}^a \neq \emptyset$, and

$$E_{4n}^\pm(a) = \tilde{\lambda}_n^\pm + \frac{a^2}{9M_n^\pm} + O(a^4), \quad \text{if } \tilde{\gamma}_n \neq \emptyset, \quad (1.36)$$

$$E_{4n}^\pm(a) = \tilde{\lambda}_n^\pm \pm \frac{\sqrt{2}a}{3\sqrt{|F''(\tilde{\lambda}_n^\pm)|}} + O(a^2), \quad \text{if } \tilde{\gamma}_n = \emptyset, \quad (1.37)$$

$$E_{4n-2}^\pm(a) = \eta_n \pm \frac{a}{3|F'(\eta_n)|} + O(a^2) \quad (1.38)$$

as $a \rightarrow 0$.

Schrödinger operator on graphs is a subject of intensive studies in the last years (see [BGP], [KL], [KS], [KuP],...). In [BGP] the magnetic Schrödinger operator on the planar square lattice was considered. The spectrum of operator is expressed in terms of the Lyapunov function of the corresponding Hill operator. In [P] these results are extended to the case of an arbitrary connected 3D graph with identical edges and the same even potential.

Schrödinger operators on nanotubes have attracted a lot of attention recently (see [KL], [KL1], [KuP],...). Authors of [KuP] consider the case of the zigzag, armchair and chiral nanotubes with even potentials q . They show that the spectrum of the operator, as a set, coincides with the spectrum of the Hill operator. Note that these results can be obtained from the results of [P] (K.Pankrashkin, non-published). In some sense the case of even potentials q is closed to the case $q = 0$. Indeed, if q is even, then $F_- = 0$ [MW] and by Theorem 1.2, the corresponding Lyapunov functions are expressed in terms of the Lyapunov function F for the Hill operator. Using the identity $F(\lambda) = \cos \kappa(\lambda)$, where $\kappa(\lambda)$ is a quasimomentum for the Hill operator, the Lyapunov function is expressed in terms of $\cos \kappa(\lambda)$, which is similar to the case $q = 0$, where $F(\lambda) = \cos \sqrt{\lambda}$.

The detailed description of spectrum of Schrödinger operator and magnetic Schrödinger operator on zigzag nanotube with arbitrary potentials was given in the articles [KL], [KL1],

[K1]. The operator was represented as the direct sum of quasi one-dimensional operators. Research of the spectrum of these quasi one-dimensional operators is based on the analysis of the monodromy matrix (see [BBK], [CK]). Authors of [KL] describe all eigenfunctions with the same eigenvalue. They define a Lyapunov function, which is analytic on some Riemann surface. On each sheet, the Lyapunov function has the same properties as in the scalar case, but it has branch points (resonances). They prove that all resonances are real and they determine the asymptotics of the periodic and anti-periodic spectrum and of the resonances at high energy. They show that there exist two types of gaps: i) stable gaps, where the endpoints are periodic and anti-periodic eigenvalues, ii) unstable (resonance) gaps, where the endpoints are resonances (i.e., real branch points of the Lyapunov function). They describe all finite gap potentials. They show that the mapping: potential \rightarrow all eigenvalues is a real analytic isomorphism for some class of potentials.

In [KL1] authors describe how the spectrum depends on the magnetic field. They observe so-called localization of the spectrum for some values of the magnetic field, when the spectrum of the operator become pure point. This phenomenon is typical for quantum graphs and was discussed in many papers (see ref. in [P1]).

Korotyaev [K1] considers the effective masses for zigzag nanotubes in magnetic fields. Following [KL], [KL1], he consider so called modified Lyapunov function and the corresponding quasimomentum. The modified Lyapunov function is entire, then the quasimomentum is an analytic function in \mathbb{C}_+ . As for the case of Hill operator, the quasimomentum is a conformal mapping of \mathbb{C}_+ onto the domain $\text{Re } k > 0, \text{Im } k > 0$ with vertical slits. Identities and a priori estimates of gap lengths, heights of slits in terms of effective masses are obtained. These values as functions of magnetic field are described.

Schrödinger operator on armchair nanotube with arbitrary potentials was considered in [BBKL], [BBK1]. In [BBKL] all eigenfunctions of the operator with the same eigenvalue are described. The Lyapunov function is analytic on some Riemann surface and has branch points (resonances). Some example is considered in this paper, which shows that there are real and non-real resonances. The detailed analysis of the spectrum is a subject of the article [BBK1]. There exist different types of gaps: i) periodic (antiperiodic) gaps, where the endpoints are periodic (antiperiodic) eigenvalues, ii) resonance gaps, where the endpoints are resonances, iii) r-mix gaps, where one endpoint is an antiperiodic eigenvalue and other endpoint is a resonance, iv) p-mix gaps, where one endpoint is an antiperiodic eigenvalue and other endpoint is a periodic eigenvalue. Asymptotics of the gaps at high energy are obtained.

We present the plan of the paper. In Section 2 we prove Theorems 1.1, 1.2 and Theorem 2.2 about the eigenfunctions. In Section 3 we prove the main Theorems 1.3-1.6. Furthermore, in this Section we prove Theorems 3.4, 3.6, where we give the detail analysis of the spectrum including the multiplicity, description of endpoints of gaps etc. Moreover, in this Section we prove an existence of gaps independent on the magnetic field for some specific potentials (see Proposition 3.5).

2 Spectrum of the operators H_k^a

We need the following result.

Lemma 2.1. *Each function $a_\omega(t) = (\mathcal{A}(\mathbf{r}_\omega + t\mathbf{e}_\omega), \mathbf{e}_\omega) = a_j$, $\omega = (n, j, k) \in \mathcal{Z}$, $t \in [0, 1]$, where*

$$a_1 = a_3 = -a_5 = a_6 = \frac{bR^2}{2} \sin(\beta - \alpha) = \frac{b(R_2 - R_1)}{4}, \quad a_2 = a_4 = \frac{bR^2}{2} \sin 2\alpha = \frac{bR_2}{4}. \quad (2.1)$$

Proof. Identity $\mathcal{A}(\mathbf{r}) = \frac{b}{2}[\mathbf{e}_3, \mathbf{r}]$, $\mathbf{e}_3 = (0, 0, 1)$, $\mathbf{r} \in \mathbb{R}^3$ yields

$$a_\omega(t) = \frac{b}{2}([\mathbf{e}_3, \mathbf{r}_\omega + t\mathbf{e}_\omega], \mathbf{e}_\omega) = \frac{b}{2}([\mathbf{e}_3, \mathbf{r}_\omega], \mathbf{e}_\omega) = a_\omega(0) = a_\omega, \quad \text{any } t \in [0, 1]. \quad (2.2)$$

Moreover, the vector field $\mathcal{A}(\mathbf{r})$ is parallel to the plane $x_3 = 0$ (this plane is orthogonal to the axis of the cylinder \mathcal{C}) and $\mathcal{A}(\mathbf{r})$ is tangential to the cylinder surface $x_1^2 + x_2^2 = R^2$. We deduce that each projection $a_\omega, \omega \in \mathcal{Z}$ of $\mathcal{A}(\mathbf{r})$ to the edge Γ_ω satisfies $a_\omega = a_j$ and $a_1 = a_3 = -a_5 = a_6, a_2 = a_4$.

We have $\mathbf{e}_{0,j,k} = \mathbf{r}_{0,j+1,k} - \mathbf{r}_{0,j,k}$, $j = 1, 2$, which yields

$$a_{0,j,k} = \frac{b}{2}([\mathbf{e}_3, \mathbf{r}_{0,j,k}], \mathbf{r}_{0,j+1,k}).$$

If $j = 1$, then $\mathbf{r}_{0,1,k} = R(c_{2k}, s_{2k}, 0)$, $\mathbf{r}_{0,2,k} = h\mathbf{e}_3 + R(\cos \zeta_k, \sin \zeta_k, 0)$ and thus

$$a_1 = a_{0,1,k} = \frac{bR^2}{2} \det \begin{pmatrix} \cos \zeta_k & \sin \zeta_k & 0 \\ 0 & 0 & 1 \\ c_{2k} & s_{2k} & 0 \end{pmatrix} = \frac{bR^2}{2} \sin(\zeta_k - \phi_{2k}) = \frac{bR^2}{2} \sin(\beta - \alpha).$$

If $j = 2$, then $\mathbf{r}_{0,3,k} = h\mathbf{e}_3 + R(c_{2k+1}, s_{2k+1}, 0)$ and thus

$$a_2 = a_{0,2,k} = \frac{bR^2}{2} \det \begin{pmatrix} c_{2k+1} & s_{2k+1} & 0 \\ 0 & 0 & 1 \\ \cos \zeta_k & \sin \zeta_k & 0 \end{pmatrix} = \frac{bR^2}{2} \sin(\phi_{2k+1} - \zeta_k) = \frac{bR^2}{2} \sin 2\alpha,$$

since $\phi_{2k+1} - \zeta_k = \frac{\pi}{N} - \beta + \alpha = 2\alpha$, which yields (2.1). ■

Now we will prove Theorem 1.1 and the identities

$$\text{Tr } \mathcal{M}_0 = 2(9F^2 - F_-^2 - 1), \quad \text{Tr } \mathcal{M}_k = \text{Tr } \mathcal{M}_0 - 4s_k^2, \quad (2.3)$$

$$\text{Tr } \mathcal{M}_0^2 = 72F^2 + \frac{1}{2}(\text{Tr } \mathcal{M}_0)^2 - 4, \quad \text{Tr } \mathcal{M}_k^2 = \text{Tr } \mathcal{M}_0^2 - 8s_k^2 \text{Tr } \mathcal{M}_0 - 16s_k^2 c_k^2. \quad (2.4)$$

Proof of Theorem 1.1 and identities (2.3), (2.4). (i) Introduce the unitary operator \mathcal{U} in $L^2(\Gamma^N)$ by $(\mathcal{U}f)_\omega = e^{ita_\omega} f_\omega$, $f = (f_\omega)_{\omega \in \mathcal{Z}}$, where a_ω is given by (2.1). We define a modified operator $H^a = \mathcal{U}^* \mathcal{H}_B \mathcal{U}$ in $L^2(\Gamma^N)$. Then H^a is given by $(H^a f)_\omega = -f''_\omega + qf_\omega$, $\omega \in \mathcal{Z}$, where

$f \in \mathfrak{D}(H^a)$. The domain $\mathfrak{D}(H^a)$ consists of the functions $f = (f_\omega)_{\omega \in \mathcal{Z}}, (f''_\omega)_{\omega \in \mathcal{Z}} \in L^2(\Gamma^N)$ and f satisfies **the Modified Kirchhoff Boundary Conditions**:

$$\begin{aligned} e^{ia_1} f_{\omega_1}(1) &= f_{\omega_2}(0) = f_{\omega_5}(0), & e^{ia_2} f_{\omega_2}(1) &= f_{\omega_3}(0) = f_{\omega_6}(0), \\ e^{ia_1} f_{\omega_3}(1) &= f_{\omega_4}(0) = e^{ia_1} f_{n-1,6,k}(1), & e^{ia_2} f_{\omega_4}(1) &= f_{n,1,k+1}(0) = e^{-ia_1} f_{n-1,5,k+1}(1), \end{aligned} \quad (2.5)$$

$$\begin{aligned} f'_{\omega_2}(0) - e^{ia_1} f'_{\omega_1}(1) + f'_{\omega_5}(0) &= 0, & f'_{\omega_3}(0) - e^{ia_2} f'_{\omega_2}(1) + f'_{\omega_6}(0) &= 0, \\ -e^{ia_1} f'_{\omega_3}(1) + f'_{\omega_4}(0) - e^{ia_1} f'_{n-1,6,k}(1) &= 0, & -e^{ia_2} f'_{\omega_4}(1) + f'_{n,1,k+1}(0) - e^{-ia_1} f'_{n-1,5,k+1}(1) &= 0, \end{aligned} \quad (2.6)$$

for all $\omega_j = (n, j, k), j = \mathbb{N}_6, (n, k) \in \mathbb{Z} \times \mathbb{Z}_N$.

Define the operator \mathcal{S} in \mathbb{C}^N by $\mathcal{S}u = (u_N, u_1, \dots, u_{N-1})^\top, u = (u_n)_1^N \in \mathbb{C}^N$. The unitary operator \mathcal{S} has the form $\mathcal{S} = \sum_1^N s^k \mathcal{P}_k$, where $\mathcal{S}e_k = s^k e_k, e_k = \frac{1}{N^{\frac{1}{2}}}(1, s^{-k}, s^{-2k}, \dots, s^{-kN+k})$ is an eigenvector (recall $s = e^{i\frac{2\pi}{N}}$); $\mathcal{P}_k u = e_k(u, e_k)$ is a projector. The function f in the Kirchhoff boundary conditions (2.5) is a vector function $f = (f_\omega), \omega = (n, j, k) \in \mathcal{Z}$. We define a new vector-valued function $f_{n,j} = (f_{n,j,k})_{k=1}^N \in \mathbb{C}^N, (n, j) \in \mathcal{Z}_1 = \mathbb{Z} \times \mathbb{N}_6$, which satisfies the equation $-f''_{n,j} + qf_{n,j} = \lambda f_{n,j}$, and the conditions

$$\begin{aligned} e^{ia_1} f_{n,1}(1) &= f_{n,2}(0) = f_{n,5}(0), & e^{ia_2} f_{n,2}(1) &= f_{n,3}(0) = f_{n,6}(0), \\ e^{ia_1} f_{n,3}(1) &= f_{n,4}(0) = e^{ia_1} f_{n-1,6}(1), & e^{ia_2} \mathcal{S} f_{n,4}(1) &= f_{n,1}(0) = e^{-ia_1} f_{n-1,5}(1), \end{aligned} \quad (2.7)$$

$$\begin{aligned} e^{ia_1} f'_{n,1}(1) - f'_{n,2}(0) - f'_{n,5}(0) &= 0, & e^{ia_2} f'_{n,2}(1) - f'_{n,3}(0) - f'_{n,6}(0) &= 0, \\ e^{ia_1} f'_{n,3}(1) - f'_{n,4}(0) + e^{ia_1} f'_{n-1,6}(1) &= 0, & e^{ia_2} \mathcal{S} f'_{n,4}(1) - f'_{n,1}(0) + e^{-ia_1} f'_{n-1,5}(1) &= 0, \end{aligned} \quad (2.8)$$

for all $n \in \mathbb{Z}$, which follow from the Kirchhoff conditions (1). The operators \mathcal{S} and \mathcal{H}_B commute, then we deduce that $\mathcal{H}_B \mathcal{P}_k$ is unitarily equivalent to the operator H_k^a acting in $L^2(\Gamma^1)$ and H_k^a is given by $(H_k^a f)_\alpha = -f''_\alpha + q(t)f_\alpha$, where $(f_\alpha)_{\alpha \in \mathcal{Z}_1}, (f''_\alpha)_{\alpha \in \mathcal{Z}_1} \in L^2(\Gamma^1)$ and components f_α satisfy the boundary conditions (1.4), (1.5). Thus \mathcal{H}_B is unitarily equivalent to the operator $H^a = \oplus_1^N H_k^a$.

Proof of (ii) and (2.3), (2.4) repeats the arguments from [BBKL]. ■

Define the subspace $\mathcal{H}_k^a(\lambda) = \{\psi \in \mathfrak{D}(H_k^a) : H_k^a \psi = \lambda \psi\}$ for $(\lambda, k) \in \sigma_{pp}(H_k^a) \times \mathbb{Z}_N$.

Theorem 2.2. *Let $(a, \lambda, k) \in \mathbb{R} \times \sigma_D \times \mathbb{Z}_N$. Then*

- i) *Every eigenfunction of $\mathcal{H}_k^a(\lambda)$ vanishes at all vertices of Γ^1 .*
- ii) *There exist the functions $\psi^{(0,\nu)} = (\psi_\alpha^{(0,\nu)})_{\alpha \in \mathcal{Z}_1} \in \mathcal{H}_k^a(\lambda), \nu \in \mathbb{N}_2$ on Γ^1 such that $\text{supp } \psi^{(0,\nu)} \subset \cup_{\ell=0,1} (\cup_{j \in \mathbb{N}_6} \Gamma_{\ell,j})$, each function $\psi^{(n,\nu)} = (\psi_{m,j}^{(n,\nu)})_{(m,j) \in \mathcal{Z}_1} = (\psi_{m-n,j}^{(0,\nu)})_{(m,j) \in \mathcal{Z}_1} \in \mathcal{H}_k^a(\lambda), n \in \mathbb{Z}$. Moreover, each $f \in \mathcal{H}_k^a(\lambda)$ satisfies:*

$$f = \sum_{(n,\nu) \in \mathbb{Z} \times \mathbb{N}_2} \widehat{f}_{n,\nu} \psi^{(n,\nu)}, \quad (\widehat{f}_{n,1}, \widehat{f}_{n,2})_{n \in \mathbb{Z}} \in \ell^2 \oplus \ell^2, \quad (2.9)$$

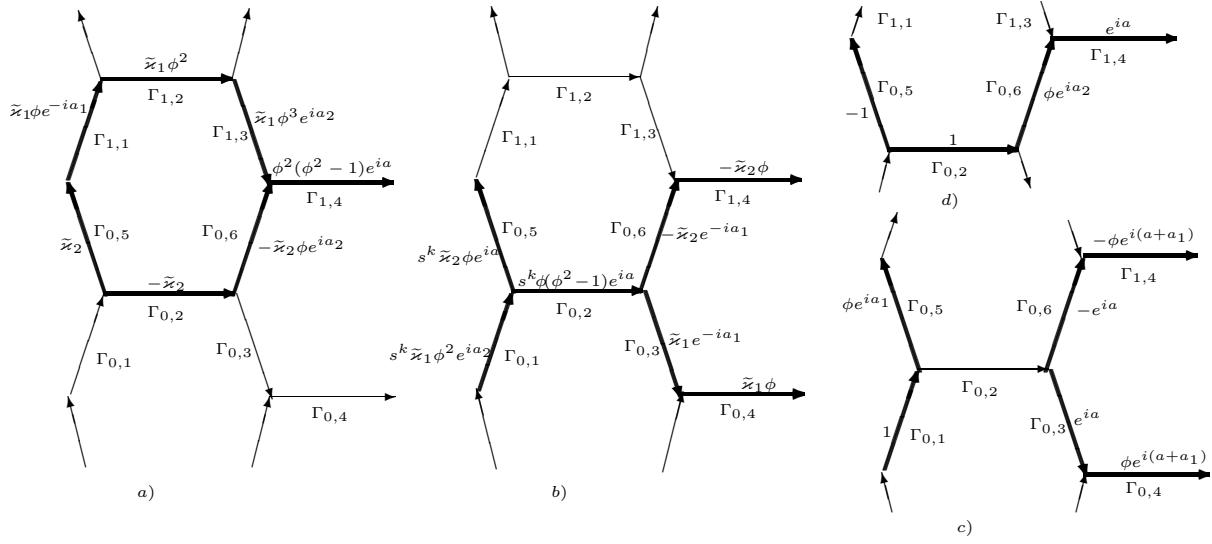


Figure 4: The supports of eigenfunctions: a) $\psi^{(0,1)}$, b) $\psi^{(0,2)}$ for $(s_k, \phi^2) \neq (0, 1)$, c) $\psi^{(0,1)}$, d) $\psi^{(0,2)}$ for $(s_k, \phi^2) = (0, 1)$; $\psi_{n,j}^{(0,\nu)} = C_{n,j}^{(0,\nu)} \varphi$, where each $C_{n,j}^{(0,\nu)}$ is written near the corresponding edge

where if $(s_k, \phi^2) = (0, 1)$, $\phi = \varphi'_1(\lambda)$, then

$$\hat{f}_{n,1} = f'_{n,1}(0), \quad \hat{f}_{n,2} = f'_{n,2}(0), \quad (2.10)$$

if $(s_k, \phi^2) \neq (0, 1)$, then

$$\hat{f}_{n,1} = \frac{f'_{n,5}(0) + s^k \phi e^{i(a+a_1)} f'_{n,6}(0)}{\tilde{\varkappa}_1 \tilde{\varkappa}_2}, \quad \hat{f}_{n,2} = -\frac{e^{ia_1} f'_{n,6}(0) + \phi e^{ia} f'_{n,5}(0)}{\tilde{\varkappa}_1 \tilde{\varkappa}_2}, \quad (2.11)$$

$\tilde{\varkappa}_1 = 1 - s^k e^{2ia} \phi^2 \neq 0$, $\tilde{\varkappa}_2 = 1 - s^k e^{2ia} \phi^4 \neq 0$. Moreover, the mapping $f \rightarrow (\hat{f}_{n,1}, \hat{f}_{n,2})_{n \in \mathbb{Z}}$ is a linear isomorphism between $\mathcal{H}_k^a(\lambda)$ and $\ell^2 \oplus \ell^2$.

Proof. Proof of i) repeats the arguments from [KL].

ii) We will define the eigenfunctions of H_k^a (see Fig.4). If $(s_k, \phi^2) \neq (0, 1)$, then $\tilde{\varkappa}_1 \neq 0$, $\tilde{\varkappa}_2 \neq 0$ and the function $\psi^{(0,1)}$ is given by

$$\begin{aligned} \psi_{n,j}^{(0,1)} &= 0 \text{ for all } (n, j) \in (\mathbb{Z} \setminus \{0, 1\}) \times \mathbb{N}_6, \text{ and } \psi_{0,j}^{(0,1)} = 0, j = 1, 3, 4, \psi_{1,j}^{(0,1)} = 0, j = 5, 6, \\ \psi_{1,4}^{(0,1)} &= \phi^2(\phi^2 - 1)e^{ia} \varphi, \quad \frac{\psi_{1,1}^{(0,1)}}{\phi e^{-ia_1}} = \frac{\psi_{1,2}^{(0,1)}}{\phi^2} = \frac{\psi_{1,3}^{(0,1)}}{\phi^3 e^{ia_2}} = \tilde{\varkappa}_1 \varphi, \quad \psi_{0,5}^{(0,1)} = -\psi_{0,2}^{(0,1)} = -\frac{\psi_{0,6}^{(0,1)}}{\phi e^{ia_2}} = \tilde{\varkappa}_2 \varphi, \end{aligned} \quad (2.12)$$

the function $\psi^{(0,2)}$ is given by

$$\begin{aligned} \psi_{n,j}^{(0,2)} &= 0, \text{ for all } (n, j) \in (\mathbb{Z} \setminus \{0, 1\}) \times \mathbb{N}_6, \text{ and } \psi_{1,j}^{(0,2)} = 0, j \neq 4, \psi_{0,2}^{(0,2)} = s^k \phi(\phi^2 - 1)e^{ia} \varphi, \\ \frac{\psi_{0,4}^{(0,2)}}{\phi} &= \frac{\psi_{0,3}^{(0,2)}}{e^{-ia_1}} = \frac{\psi_{0,1}^{(0,2)}}{s^k \phi^2 e^{ia_2}} = \tilde{\varkappa}_1 \varphi, \quad -\frac{\psi_{1,4}^{(0,2)}}{\phi} = -\frac{\psi_{0,6}^{(0,2)}}{e^{-ia_1}} = \frac{\psi_{0,5}^{(0,2)}}{s^k \phi e^{ia}} = \tilde{\varkappa}_2 \varphi. \end{aligned} \quad (2.13)$$

If $(s_k, \phi^2) = (0, 1)$, then $\tilde{\alpha}_1 = \tilde{\alpha}_2 = 0$ and the functions $\psi^{(0,\nu)}$ are given by

$$\begin{aligned} \psi_{n,j}^{(0,\nu)} &= 0, \quad (n, j) \in (\mathbb{Z} \setminus \{0, 1\}) \times \mathbb{N}_6, \quad \psi_{1,j}^{(0,\nu)} = 0, \quad j \in \mathbb{N}_6 \setminus \{4\}, \\ \psi_{0,1}^{(0,1)} &= \phi e^{-ia_1} \psi_{0,5}^{(0,1)} = -e^{-ia} \psi_{0,6}^{(0,1)} = e^{-ia} \psi_{0,3}^{(0,1)} = \varphi, \quad -\psi_{1,4}^{(0,1)} = \psi_{0,4}^{(0,1)} = \phi e^{i(a+a_1)} \varphi, \quad \psi_{0,1}^{(0,2)} = 0, \\ \psi_{0,1}^{(0,2)} &= \psi_{0,3}^{(0,2)} = \psi_{0,4}^{(0,2)} = 0, \quad \psi_{0,2}^{(0,2)} = -\psi_{0,5}^{(0,2)} = e^{-ia} \psi_{1,4}^{(0,2)} = e^{-ia_2} \phi \psi_{0,6}^{(0,2)} = \varphi. \end{aligned} \quad (2.14)$$

Using (2)-(2), we deduce that $\psi^{(0,\nu)}$ satisfy the Kirchhoff conditions (1.4), (1.5). Thus $\psi^{(0,\nu)}$ are eigenfunctions of H_k^a . The operator H_k^a is periodic, then each $\psi^{(n,\nu)}$, $(n, \nu) \in \mathbb{Z} \times \mathbb{N}_2$ is an eigenfunction. We will show that the sequence $\psi^{(n,\nu)}$, $(n, \nu) \in \mathbb{Z} \times \mathbb{N}_2$ forms a basis for $\mathcal{H}_k^a(\lambda)$. Let $h = \sum_{(n,\nu) \in \mathbb{Z} \times \mathbb{N}_2} \alpha_{n,\nu} \psi^{(n,\nu)} = 0$. Then (2), (2) imply for $(s_k, \phi^2) \neq (0, 1)$

$$0 = h|_{\Gamma_{n,5}} = (\alpha_{n,1} + \alpha_{n,2} s^k \phi e^{ia}) \tilde{\alpha}_2 \varphi, \quad 0 = h|_{\Gamma_{n,6}} = -(\alpha_{n,1} \phi e^{ia} + \alpha_{n,2}) \tilde{\alpha}_2 e^{-ia_1} \varphi, \quad n \in \mathbb{Z},$$

which yields $\alpha_{n,\nu} = 0$ for all $(n, \nu) \in \mathbb{Z} \times \mathbb{N}_2$. Hence $\psi^{(n,\nu)}$ are linearly independent. The similar arguments show that $\psi^{(n,\nu)}$ are linearly independent for $(s_k, \phi^2) = (0, 1)$.

For any $f \in \mathcal{H}_k^a(\lambda)$ we will show the identity (2.9), i.e.,

$$f = \hat{f}, \quad \text{where } \hat{f} = \sum_{(n,\nu) \in \mathbb{Z} \times \mathbb{N}_2} \hat{f}_{n,\nu} \psi^{(n,\nu)} \quad \text{and} \quad \hat{f}_{n,\nu} \quad \text{are given by (2.11).} \quad (2.15)$$

From $\lambda \in \sigma_D$, we deduce that $f|_{\Gamma_{n,j}} = f'_{n,j}(0) \varphi$. If $(s_k, \phi^2) \neq (0, 1)$, then identities (2.11)-(2) provide for all $n \in \mathbb{Z}$

$$\begin{aligned} \hat{f}|_{\Gamma_{n,5}} &= \sum_{(\ell,\nu) \in \mathbb{Z} \times \mathbb{N}_2} \hat{f}_{\ell,\nu} \psi^{(\ell,\nu)}|_{\Gamma_{n,5}} = (\hat{f}_{n,1} + \hat{f}_{n,2} s^k \phi e^{ia}) \tilde{\alpha}_2 \varphi = f'_{n,5}(0) \varphi = f|_{\Gamma_{n,5}}, \\ \hat{f}|_{\Gamma_{n,6}} &= \sum_{(\ell,\nu) \in \mathbb{Z} \times \mathbb{N}_2} \hat{f}_{\ell,\nu} \psi^{(\ell,\nu)}|_{\Gamma_{n,6}} = -(\hat{f}_{n,1} \phi e^{ia} + \hat{f}_{n,2}) \tilde{\alpha}_2 e^{-ia_1} \varphi = f'_{n,6}(0) \varphi = f|_{\Gamma_{n,6}}. \end{aligned} \quad (2.16)$$

If $(s_k, \phi^2) = (0, 1)$, then identities (2.10),(2) give for all $n \in \mathbb{Z}$

$$\hat{f}|_{\Gamma_{n,1}} = \hat{f}_{n,1} \varphi = f'_{n,1}(0) \varphi = f|_{\Gamma_{n,1}}, \quad \hat{f}|_{\Gamma_{n,2}} = \hat{f}_{n,2} \varphi = f'_{n,2}(0) \varphi = f|_{\Gamma_{n,2}}. \quad (2.17)$$

Identities (2.16), (2.17) yield $\sum |\hat{f}_{n,\nu}|^2 < \infty$ and $\hat{f} \in L^2(\Gamma^1)$, since $f \in L^2(\Gamma^1)$.

Note that \hat{f} satisfies the Kirchhoff conditions (1.4), (1.5) and $-\hat{f}''_\alpha + q\hat{f}_\alpha = \lambda \hat{f}_\alpha$, $\alpha \in \mathcal{Z}_1$. Consider the function $u = f - \hat{f}$. The function $u = 0$ at all vertices of Γ^1 and then $u_{n,j} = C_{n,j} \varphi$, $(n, j) \in \mathbb{Z} \times \mathbb{N}_6$. If $(s_k, \phi^2) \neq (0, 1)$, then (2.16) gives $C_{n,5} = C_{n,6} = 0$. Let $n \in \mathbb{Z}$ and assume that $C_{n,1} = C$. Then the Kirchhoff boundary conditions (1.4)-(1.5) yield $C_{n,2} = C \phi e^{ia_1}$, $C_{n,3} = C \phi^2 e^{ia}$, $C_{n,4} = C \phi^3 e^{i(a+a_1)}$, $C_{n,1} = C s^k \phi^4 e^{2ia}$. Since $C_{n,1} = C$, we obtain $C = 0$ and $u = 0$, which yields (2.15). If $(s_k, \phi^2) = (0, 1)$, then (2.17) gives $C_{n,1} = C_{n,2} = 0$. The Kirchhoff boundary conditions (1.4)-(1.5) yield $C_{n,5} = 0$, and then $C_{n,4} = 0$, $n \in \mathbb{Z}$. Assume that $C_{n,3} = C$. Then $C_{n,6} = -C_{0,3} = -C$ and $C_{n+1,3} = -C_{n,6} = C$ for all $n \in \mathbb{Z}$. Due to $u \in L^2(\Gamma^1)$, we have $C = 0$ and $u = 0$, which yields (2.15).

The mapping $f \rightarrow (\widehat{f_{n,\nu}})_{(n,\nu) \in \mathbb{Z} \times \mathbb{N}_2}$ is a linear and one-to-one mapping from \mathcal{H}_k^a onto $\ell^2 \oplus \ell^2$. Then it is a linear isomorphism. ■

Proof of Theorem 1.2. (i) Using the arguments from [BBK],[KL] and identities (1.10), (2.3), (2.4) we obtain (1.12), (1.13).

(ii), (iii) Proof of the statements and identities (1.15) repeats the corresponding arguments from [KL]. Identities (1.12), (1.17) yield $F_{k,\nu}(\cdot, -a) = F_{N-k,\nu}(\cdot, a)$, $F_{k,\nu}(\cdot, a + \frac{\pi}{N}) = F_{k+1,\nu}(\cdot, a)$, $(\nu, k) \in \mathbb{N}_2 \times \mathbb{Z}_N$. Then identities (1.15) yield (1.16). By Theorem 2.2, each point $\lambda_0 \in \sigma_{pp}(H_k^a)$ has an infinite multiplicity. ■

Lemma 2.3. *Let $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$. Then there exists an integer $n_0 > 1$ such that*

(i) *The function $D_k^- = D_0^- = \det(\mathcal{M}_k + I_4)$ has exactly $4n_0$ zeros, counted with multiplicities, in the domain $\{\lambda : |\sqrt{\lambda}| < \pi n_0\}$ and for each $n > n_0$, exactly two zeros, counted with multiplicities, in each domain $\{\lambda : |\sqrt{\lambda} - \pi n - \frac{\pi}{2} \pm \arcsin \frac{1}{3}| < \frac{1}{3}\}$. There are no other zeros.*

(ii) *Each function $D_k^+ = \det(\mathcal{M}_k - I_4)$, $k \in \mathbb{Z}_N$ has exactly $4n_0 + 2$ zeros, counted with multiplicities, in the domain $\{\lambda : |\sqrt{\lambda}| < \pi n_0 + \frac{\pi}{2}\}$, and for each $n > n_0$ exactly one simple zero in each domain $\{\lambda : |\sqrt{\lambda} - \pi n \pm \arccos \frac{\sqrt{5-4c_k}}{3}| < \frac{1}{3}\}$, exactly one simple zero in each domain $\{\lambda : |\sqrt{\lambda} - \pi n \pm \arccos \frac{\sqrt{5+4c_k}}{3}| < \frac{s_k}{3}\}$, if $s_k \neq 0$, and exactly two zeros, counted with multiplicities, in each domain $\{\lambda : |\sqrt{\lambda} - \pi n \pm \arccos \frac{\sqrt{5+4c_k}}{3}| < \frac{1}{3}\}$, if $s_k = 0$. There are no other zeros.*

(iii) *Let $c_k \neq 0, s_k \neq 0$. Then the function ρ_k has exactly $2n_0$ zeros, counted with multiplicities, in the domain $\{\lambda : |\sqrt{\lambda}| < \pi n_0\}$, and for each $n > n_0$ exactly one simple real zero in each domain $\{\lambda : |\sqrt{\lambda} - (\pi n - \frac{\pi}{2} \pm \arcsin \frac{s_k}{3})| < \frac{s_k}{3}\}$. There are no other zeros.*

Proof. Proof uses the Rouché theorem and repeats the arguments from [KL]. ■

Below we need some identities for D_k^\pm . Substituting (1.12) into (1.18) we obtain

$$D_k^+ = (9F^2 - g_{k,1})(9F^2 - g_{k,2}), \quad D_k^- = D_0^- = (9F^2 - h_1)(9F^2 - h_2) \quad \text{on } \mathbb{R}, \quad (2.18)$$

where

$$g_{k,\nu} = 5 + F_-^2 + (-1)^\nu 2\sqrt{F_-^2 + 4c_k^2}, \quad h_\nu = (1 + (-1)^\nu |F_-|)^2, \quad (\nu, k) \in \mathbb{N}_2 \times \mathbb{Z}_N. \quad (2.19)$$

Lemma 2.4. *Let $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$. Then*

(i) *For all $(\nu, n) \in \mathbb{N}_2 \times \mathbb{N}$ the periodic and antiperiodic eigenvalues satisfy*

$$\lambda_{\nu,n-1}^{k,\pm}(a) = \lambda_{\nu,n-1}^{N-k,\pm}(-a), \quad \lambda_{\nu,p}^{k,\pm}(a) = \lambda_{\nu,p}^{0,\pm}(0), \quad \gamma_{\nu,p}^k(a) = \gamma_{\nu,p}^0(0), \quad \gamma_{1,p}^0 = \varkappa_n, \quad p = 2n - 1, \quad (2.20)$$

$$\begin{aligned} \widetilde{\lambda}_{n-1}^+ &\leq \lambda_{2,p-1}^{k,+} \leq \min\{\lambda_{2,p}^{0,-}, \lambda_{1,p-1}^{k,+}\} \leq \max\{\lambda_{2,p}^{0,-}, \lambda_{1,p-1}^{k,+}\} \leq \lambda_{1,p}^{0,-} \\ &\leq \eta_n \leq \lambda_{1,p}^{0,+} \leq \min\{\lambda_{1,p+1}^{k,-}, \lambda_{2,p}^{0,+}\} \leq \max\{\lambda_{1,p+1}^{k,-}, \lambda_{2,p}^{0,+}\} \leq \lambda_{2,p+1}^{k,-} \leq \widetilde{\lambda}_n^-, \end{aligned} \quad (2.21)$$

$$\lambda_{2,p}^{0,-} < \lambda_{1,p-1}^{k,+} \Leftrightarrow u_k(\lambda_{2,p}^{0,-}) > 0; \quad \lambda_{2,p}^{0,+} > \lambda_{1,p+1}^{k,-} \Leftrightarrow u_k(\lambda_{2,p}^{0,+}) > 0, \quad (2.22)$$

$$\cup_{n \geq 1} \gamma_{\nu,2n-1}^0 = \{\lambda \in \mathbb{R} : 9F^2(\lambda) < h_\nu(\lambda)\}, \quad \cup_{n \geq 0} \gamma_{\nu,2n}^k = \{\lambda \in \mathbb{R} : 9F^2(\lambda) > g_{k,\nu}(\lambda)\}, \quad (2.23)$$

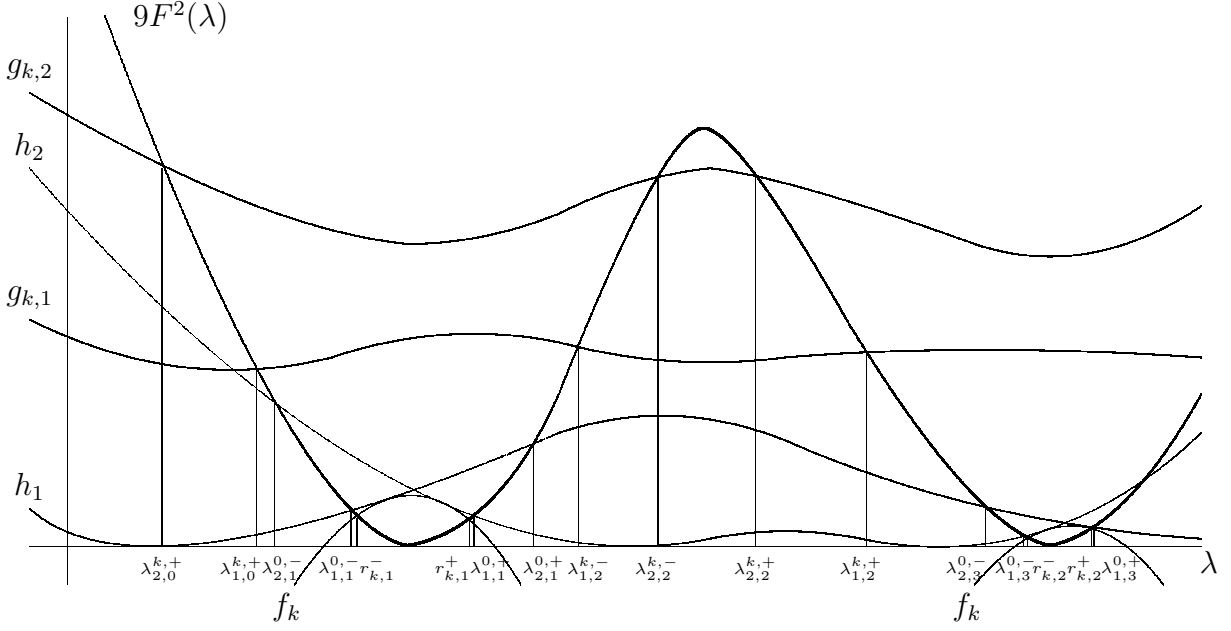


Figure 5: Functions $9F^2$, g_k^\pm , h^\pm and f_k

where

$$\gamma_{\nu,0}^k = (-\infty, \lambda_{\nu,0}^{k,+}), \quad \gamma_{\nu,n}^k = (\lambda_{\nu,n}^{k,-}, \lambda_{\nu,n}^{k,+}), \quad (\nu, n) \in \mathbb{N}_2 \times \mathbb{N}.$$

(ii) If $s_k^2(a) < s_\ell^2(a_1)$ for some $(a_1, \ell) \in \mathbb{R} \times \mathbb{Z}_N$, then for all $n \geq 1$

$$\lambda_{2,2n-2}^{k,+}(a) < \lambda_{2,2n-2}^{\ell,+}(a_1), \quad \lambda_{1,2n-2}^{\ell,+}(a_1) < \lambda_{1,2n-2}^{k,+}(a), \quad \lambda_{1,2n}^{k,-}(a) < \lambda_{1,2n}^{\ell,-}(a_1), \quad \lambda_{2,2n}^{\ell,-}(a_1) < \lambda_{2,2n}^{k,-}(a). \quad (2.24)$$

Proof. Proof uses identities (2.18) and properties of the function F and repeats the arguments from [BBK1], Lemma 2.2 (see also Fig.5). ■

3 Proof of Theorems 1.3-1.5

Let $R_k = \{\lambda \in \mathbb{R} : \rho_k(\lambda) > 0\}$, if $\rho_k \neq 0$, and $R_k = \mathbb{R}$, if $\rho_k = 0$. In Lemmas 3.1-3.3 we describe the set $\sigma_{k,\nu} = \{\lambda \in \mathbb{R} : F_{k,\nu}(\lambda) \in [-1, 1]\}$ in terms of F .

Lemma 3.1. *Let $a \in \mathbb{R}$. For all $k \in \mathbb{Z}_N$ and $\lambda \in R_k$ the following relations hold true:*

$$F_{k,\nu}(\lambda) < 1 \quad \text{iff} \quad 9F^2(\lambda) < g_{k,\nu}(\lambda), \quad \nu = 1, 2, \quad (3.1)$$

$$F_{k,1}(\lambda) > -1 \quad \text{iff} \quad \{9F^2(\lambda) > h_1(\lambda) \text{ or } |F_-(\lambda)| < c_k^2\}, \quad (3.2)$$

$$F_{k,2}(\lambda) > -1 \quad \text{iff} \quad \left\{ 9F^2(\lambda) > h_2(\lambda) \text{ or } \{9F^2(\lambda) < h_1(\lambda) \text{ and } |F_-(\lambda)| < c_k^2\} \right\}. \quad (3.3)$$

Proof. Proof repeats the arguments from [BBK1], Lemma 3.1. Using the identities (1.12), (2.19) we write the functions $F_{k,\nu}$ in terms of $g_{k,\nu}, h_\nu$ and prove (3.1)-(3.3). ■

Now we describe the zeros of ρ_k and the functions $F_{k,\nu}$ on the interval \varkappa_n .

Lemma 3.2. *Let $c_k \neq 0$ for some $(a, k) \in \mathbb{R} \times \mathbb{Z}_N$. Then*

(i) *The following relation holds true:*

$$\mathbb{R} \setminus \overline{R_k} \subset \bigcup_{n \geq 1} \varkappa_n, \quad \text{where} \quad \varkappa_n = (\lambda_{1,2n-1}^{0,-}, \lambda_{1,2n-1}^{0,+}). \quad (3.4)$$

All real zeros of ρ_k belong to the set $\bigcup_{n \geq 1} \overline{\varkappa_n}$. Each interval $\overline{\varkappa_n}, n \geq 1$ contains even number ≥ 0 of zeros of ρ_k , counted with multiplicities.

(ii) *Let $\varkappa_n \not\subset R_k$. Then for each $\sigma = \pm$ the following relations hold true:*

$$\text{sign } v_k = \text{const} \quad \text{on each} \quad \varkappa_{k,n}^\sigma \subset R_k, \quad (3.5)$$

$$\text{if } v_k(\lambda) > 0 \text{ for some } \lambda \in \varkappa_{k,n}^\sigma, \quad \text{then} \quad F_{k,2} < F_{k,1} < -1 \text{ on } \varkappa_{k,n}^\sigma, \quad (3.6)$$

$$\text{if } v_k(\lambda) < 0 \text{ for some } \lambda \in \varkappa_{k,n}^\sigma, \quad \text{then} \quad -1 < F_{k,2} < F_{k,1} \text{ on } \varkappa_{k,n}^\sigma, \quad (3.7)$$

where

$$\varkappa_{n,k}^- = (\lambda_{1,2n-1}^{0,-}, r_{k,n}^-), \quad \varkappa_{n,k}^+ = (r_{k,n}^+, \lambda_{1,2n-1}^{0,+}), \quad n \geq 1 \quad (3.8)$$

If $\varkappa_n \subset R_k$, then

$$v_k > 0 \quad \text{and} \quad F_{k,2} < F_{k,1} < -1 \quad \text{on} \quad \varkappa_n. \quad (3.9)$$

(iii) *If $v_k(\lambda) < 0$ for some $\lambda \in \overline{\varkappa_n}$, then ρ_k has even number ≥ 2 of zeros on $\overline{\varkappa_n}$.*

Proof. Proof repeats the arguments from [BBK1], Lemma 3.2. The last identity in (1.12) gives

$$\rho = c_k^2(9F^2 - f_k), \quad \text{where} \quad f_k = s_k^2 \left(1 - \frac{F_-^2}{c_k^2} \right). \quad (3.10)$$

Identities (2.19) yield $h_1 \geq f_k$. Using the properties of F we obtain (3.4) (see also Fig.5). Using (3.10), Lemma 3.1 and the more detail analysis (see [BBK1]) we obtain (3.5)-(3.9) and the statement (iii). ■

For each $(k, \nu) \in \mathbb{Z}_N \times \mathbb{N}_2$ we introduce the sets

$$\mathfrak{S}_{k,\nu} = \bigcup_{n \geq 1} \left([\lambda_{\nu,p-1}^{k,+}, \lambda_{\nu,p}^{0,-}] \cup [\lambda_{\nu,p}^{0,+}, \lambda_{\nu,p+1}^{k,-}] \right), \quad \mathfrak{S}_k^R = \bigcup_{\sigma=\pm, n \in N_\sigma} \overline{\varkappa_{k,n}^\sigma}, \quad N_\pm = \{n \in \mathbb{N} : v_k(\lambda_{1,p}^{0,\pm}) < 0\}, \quad (3.11)$$

where $p = 2n - 1$. The set $\mathfrak{S}_{k,\nu}$ is a "stable" part of $\sigma_{k,\nu} = \{\lambda \in \mathbb{R} : F_{k,\nu}(\lambda) \in [-1, 1]\}$, and \mathfrak{S}_k^R is an "unstable" part of $\sigma_{k,\nu}$ (see (3.13), (3.14)).

Lemma 3.3. *Let $(a, k, \nu) \in \mathbb{R} \times \mathbb{Z}_N \times \mathbb{N}_2$. Then the following identities hold true:*

$$\mathfrak{S}_{k,\nu} = \{\lambda \in \mathbb{R} : h_\nu(\lambda) \leq 9F^2(\lambda) \leq g_{k,\nu}(\lambda)\}, \quad (3.12)$$

$$\mathfrak{S}_k^R = \begin{cases} \{\lambda \in R_k : 9F^2(\lambda) \leq h_1(\lambda) \text{ and } v_k(\lambda) \leq 0\}, & \text{if } c_k \neq 0 \\ \emptyset, & \text{if } c_k = 0 \end{cases}, \quad (3.13)$$

$$\sigma_{k,\nu} = \mathfrak{S}_{k,\nu} \cup \mathfrak{S}_k^R. \quad (3.14)$$

Proof. Proof uses the results of Lemma 3.1 and repeats the arguments from [BBK1], Lemma 3.3. Relations (2.23) and Lemma 3.2 yield (3.12), (3.13). Then Lemma 3.1 gives (3.14). ■

Proof of Theorem 1.3. Substituting (3.11) into (3.14) and using the identity $\sigma_{ac}(H_k^a) = \sigma_{k,1} \cup \sigma_{k,2}$ we obtain (1.20), (1.21). Identities $\lambda_{\nu,p}^{k,\pm}(a) = \lambda_{\nu,p}^{0,\pm}(0)$ are proved in (2.20). Using (1.21) and the definition of \varkappa_n in (1.23) we obtain (1.22). ■

Theorem 3.4. (multiplicity of the spectrum) *Let $(a, k, n) \in [0, \frac{\pi}{2N}] \times \mathbb{Z}_N \times \mathbb{N}, p = 2n - 1$. Then the following relations hold true:*

$$\begin{aligned} E_{2,p}^{k,\pm} &= E_{2,p}^{0,\pm}, \quad E_{2,p-1}^{k,+} \leq \min\{E_{2,p}^{k,-}, E_{1,p-1}^{k,+}\} \leq \max\{E_{2,p}^{k,-}, E_{1,p-1}^{k,+}\} \leq E_{1,p}^{k,-} \\ &\leq E_{1,p}^{k,+} \leq \min\{E_{1,p+1}^{k,-}, E_{2,p}^{k,+}\} \leq \max\{E_{1,p+1}^{k,-}, E_{2,p}^{k,+}\} \leq E_{2,p+1}^{k,-}, \end{aligned} \quad (3.15)$$

$$E_{2,p}^{k,-} < E_{1,p-1}^{k,+} \quad \text{iff} \quad u_k(E_{2,p}^{k,-}) > 0; \quad E_{1,p+1}^{k,-} < E_{2,p}^{k,+} \quad \text{iff} \quad u_k(E_{2,p}^{k,+}) > 0. \quad (3.16)$$

Moreover,

- (i) If $\mathfrak{S}_k^R \neq \emptyset$, then the spectrum of H_k^a in \mathfrak{S}_k^R has multiplicity 4.
- (ii) If $\mathfrak{S}_k = \mathfrak{S}_{k,1} \cap \mathfrak{S}_{k,2} \neq \emptyset$ then the spectrum of H_k^a in \mathfrak{S}_k has multiplicity 4.
- (iii) The spectrum of H_k^a in $\sigma_{ac}(H_k^a) \setminus (\mathfrak{S}_k \cup \mathfrak{S}_k^R)$ has multiplicity 2.

Proof. Relations (1.21) and (2.21) yield (3.15). Relations (2.22) imply (3.16). Proof of the other statements repeats the arguments from [BBK1], proof of Theorem 1.2. Relations (3.7) provide the statement (i), identity (3.14) yields the statements (ii), (iii) (see [BBK1]). ■

Remark. 1) Using identities (1.21), (3.11) we deduce that $\mathfrak{S}_k^R \neq \emptyset$ iff $\{E_{1,p}^{k,\sigma} = r_{k,n}^\sigma, \varkappa_{k,n}^\sigma \neq \emptyset$ for some $(n, \sigma) \in \mathbb{N} \times \{+, -\}\}$.

2) Identities (1.21) and (3.11) show that $\mathfrak{S}_k \neq \emptyset$ iff $E_{2,p}^{k,-} > E_{1,p-1}^{k,+}$ (or $E_{1,p+1}^{k,-} > E_{2,p}^{k,+}$) for some $n \geq 1$. Relations (3.16) yields $u_k(E_{2,p}^{k,-}) > 0$ (or $u_k(E_{2,p}^{k,+}) > 0$) for this n . Then the spectrum of H_k^a in the interval $(E_{1,p-1}^{k,+}, E_{2,p}^{k,-})$ (or $(E_{2,p}^{k,+}, E_{1,p+1}^{k,-})$) has multiplicity 4.

Below we need the asymptotics from [M]

$$F(\lambda) = \cos \sqrt{\lambda} + \frac{O(e^{|\operatorname{Im} \sqrt{\lambda}|})}{\sqrt{|\lambda|}}, \quad F_-(\lambda) = \frac{O(e^{|\operatorname{Im} \sqrt{\lambda}|})}{\sqrt{|\lambda|}} \quad \text{as} \quad |\lambda| \rightarrow \infty. \quad (3.17)$$

Proof of Theorem 1.4. (i) Estimates (3.15) show that the intervals $G_{\nu,k,0} = (-\infty, E_{\nu,0}^{k,+})$, $G_{\nu,k,n} = (E_{\nu,n}^{k,-}, E_{\nu,n}^{k,+})$, $(\nu, n) \in \mathbb{N}_2 \times \mathbb{N}$, satisfy:

$$G_{1,k,0} \cap G_{2,k,m} = \emptyset \text{ for } m \notin \{0, 1\}, \quad G_{1,k,2n-1} \cap G_{2,k,m} = \emptyset \text{ for } m \neq 2n - 1,$$

$$G_{1,k,2n} \cap G_{2,k,m} = \emptyset \text{ for } m \notin \{2n - 1, 2n, 2n + 1\}.$$

Then the gaps $G_{k,n}^a, n \geq 0$ in the spectrum H_k^a satisfy

$$\begin{aligned} G_{k,0}^a &= G_{1,k,0} \cap G_{2,k,0}, \quad G_{k,2n}^a = G_{1,k,n} \cap G_{2,k,n}, \\ G_{k,4n-3}^a &= G_{1,k,2n-2} \cap G_{2,k,2n-1}, \quad G_{k,4n-1}^a = G_{1,k,2n} \cap G_{2,k,2n-1}, \end{aligned} \quad (3.18)$$

$n \geq 1$, which yields all identities in (1.24). Estimates (2.21) give all inclusions in (1.24). Relations (2.24) give (1.25).

For $(a, k) = (0, 0)$ the first identity in (1.26) is proved in [BBK1]. If $a \neq 0$, then $s_k \neq 0$. Let $c_k \neq 0$. Asymptotics (3.17) implies $F_-(\lambda) \rightarrow 0$ as $\lambda \rightarrow +\infty$. The last identities in (1.21) give $E_{1,p}^{k,\pm} = r_{k,n}^\pm$, $n \geq n_0$. By Lemma 2.3 (iii), $r_{k,n}^- < r_{k,n}^+$ for such n . Hence the intervals $G_{k,4n-2}^a \neq \emptyset$ in this case. Let $c_k = 0$. The last identities in (1.21) give $E_{1,p}^{k,\pm} = \lambda_{1,p}^{0,\pm}$, $n \geq 1$. Identities (3.11), (3.12) yield $\lambda_{1,p}^{0,\pm}$ are zeros of $9F^2 - h_1$, where h_1 is given by (2.19). We have $h_1(\lambda) \rightarrow 1$ as $\lambda \rightarrow +\infty$. The properties of F show that the function $9F^2 - h_1$ has only simple zeros on $(\lambda_0, +\infty)$ for sufficiently large $\lambda_0 > 0$. Then $\lambda_{1,p}^{0,-} < \lambda_{1,p}^{0,+}$ for all $n \geq n_0$. Hence $G_{k,4n-2}^a \neq \emptyset$ in this case, which yields the first identities in (1.26) for $(a, k) \neq (0, 0)$.

If $(a, k) \neq (0, 0)$, then $s_k \neq 0$ and estimates (3.16) give $E_{k,4n-3}^- > E_{k,4n-3}^+$ and $E_{k,4n-1}^- > E_{k,4n-1}^+$, $n > n_0$. Hence $G_{k,2n-1}^a = \emptyset$ for such k, n , which gives the second identities in (1.26). (ii) If $v_k(\lambda) > 0$ on \varkappa_n , then identities (1.21) show that $E_{1,p}^{k,\pm}(a) = \lambda_{1,p}^{0,\pm}$. Then (1.24) gives $G_{k,4n-2}^a = (E_{1,p}^{k,-}(a), E_{1,p}^{k,+}(a)) = \varkappa_n$. ■

Proof of Theorem 1.5. Using the results of Theorem 1.2 (iii) we obtain (1.27).

(i) Theorem 1.4 (i) provides $\sigma_{ac}(H^a) = \mathbb{R} \setminus \cup_{n \geq 0} G_n^a$, where $\text{gap } G_n^a = \cap_{k \in \mathbb{Z}_N} G_{k,n}^a$. The first relations in (1.25) show $G_{4n}^a = G_{0,4n}^a$, $n \geq 0$. The second relations in (1.25) imply $G_{2n-1}^a = G_{m_1,2n-1}^a$, $n \geq 1$, where $m_1 = \frac{N}{2}$ or $\frac{N-1}{2}$. The relations $G_{k,4n-2}^a \subset \varkappa_n$ give $G_{4n-2}^a \subset \varkappa_n$. The relations $\tilde{\gamma}_{n-1} \subset G_{k,4n}^a$, $\eta_n \in [E_{1,2n-1}^{k,-}, E_{1,2n-1}^{k,+}]$ give the corresponding relations $\tilde{\gamma}_n \subset G_{4n}^a$, $\eta_n \in [E_{1,2n-1}^-, E_{1,2n-1}^+]$. Thus, we have proved all relations in (1.28). Relations (1.25) yield (1.29). Relations (1.26) yield (1.30).

(ii) In order to prove asymptotics (1.31) we assume that $\int_0^1 q(t)dt = 0$. Let $m = 0$. Using the first identities in (1.21) and (1.24) we obtain $(E_{4n}^-, E_{4n}^+) = G_{4n}^a = G_{0,4n}^a = (E_{2,2n}^{0,-}, E_{2,2n}^{0,+}) = (\lambda_{2,2n}^{0,-}, \lambda_{2,2n}^{0,+})$. Identities (2.19) and Lemma 2.3 (ii) show that $E_{4n}^\pm = \lambda_{2,2n}^{0,\pm}$ are zeros of the function $9F^2 - g_{0,2}$ and $\sqrt{E_{4n}^\pm} = \pi n \pm \tilde{\theta}_0 + \varepsilon_n^\pm$, where $|\varepsilon_n^\pm| \leq \frac{1}{3}$ for large n . Let $\lambda = E_{4n}^\pm$ and $\varepsilon = \varepsilon_n^\pm$. Then (3.17) give

$$9F^2(\lambda) = 9 \cos^2(\pi n \pm \tilde{\theta}_0 + \varepsilon) + O(n^{-2}) = 5 + 4|c_0| \mp 9\varepsilon \sin(2\tilde{\theta}_0) + O(\varepsilon^2) + O(n^{-2}),$$

and $F_-(\lambda) = O(n^{-1})$ as $n \rightarrow +\infty$. Identities (2.19) imply $g_{0,2}(\lambda) = 5 + 4|c_0| + O(n^{-2})$. Then $9F^2(\lambda) - g_{0,2}(\lambda) = \mp 9\varepsilon \sin(2\tilde{\theta}_0) + O(\varepsilon^2) + O(n^{-2})$. Hence $\varepsilon = O(n^{-2})$ and $\sqrt{E_{4n}^\pm} = \pi n \pm \tilde{\theta}_0 + O(n^{-2})$, which yields (1.31) for $m = 0$.

Let $m = 1$. Identity $G_n^a = \cap_{k \in \mathbb{Z}_N} G_{k,n}^a$ and (1.24) imply $E_{4n-2}^- = \max_{k \in \mathbb{Z}_N} E_{1,2n-1}^{k,-}$, $E_{4n-2}^+ = \min_{k \in \mathbb{Z}_N} E_{1,2n-1}^{k,+}$. Identities (1.12) show that for large $n \geq 1$ the energies $E_{1,2n-1}^{k,\pm} = r_{k,2n}^\pm$ are zeros of the function $9F^2 - f_k$, where $f_k = s_k^2(1 - \frac{F^2}{c_k^2})$. By Lemma 2.3 (i), (iii), $\sqrt{E_{1,2n-1}^{k,\pm}} = \pi n - \frac{\pi}{2} \pm \theta_k + \varepsilon_n^\pm$, $\theta_k = \arcsin \frac{s_k}{3}$, where $|\varepsilon_n^\pm| \leq \frac{s_k}{3}$ for large n . Let $\lambda = E_{1,2n-1}^{k,\pm}$ and $\varepsilon = \varepsilon_n^\pm$. Then (3.17) give

$$9F^2(\lambda) = 9 \cos^2(\pi n - \frac{\pi}{2} \pm \theta_k + \varepsilon) + O(n^{-2}) = s_k^2 \pm 9\varepsilon \sin(2\theta_k) + O(\varepsilon^2) + O(n^{-2}),$$

and $F_-(\lambda) = O(n^{-1})$. Then $f_k(\lambda) = s_k^2 + O(n^{-2})$ and $9F^2(\lambda) - f_k(\lambda) = \pm 9\varepsilon \sin(2\theta_k) +$

$O(\varepsilon^2) + O(n^{-2})$. Then $\varepsilon = O(n^{-2})$, which yields $E_{1,2n-1}^{k,\pm} = (\pi n - \frac{\pi}{2} \pm \theta_k + O(n^{-2}))^2$. This asymptotics and the identity $\tilde{\theta}_1 = \min_{k \in \mathbb{Z}_N} \theta_k$ give (1.31) for $m = 1$.

(iii) Theorem 1.4 (ii) yields the statement. ■

Proof of Theorem 1.6. (i) If $q \in L_{\text{even}}^2(0, 1)$, then $F_- = 0$. Let $c_k = 0$. The last identity in (1.12) implies $\rho_k = 0$ and identity (1.19) yields $v_k = 0$. Using identities (1.21) $E_{1,p}^{k,\pm} = \lambda_{1,2n-1}^{0,\pm}$ and (1.23), (1.24) provide $G_{k,4n-2}^a = \mathcal{N}_n$. Let $c_k \neq 0$. Then (1.19) yields $v_k = -c_k^2 < 0$. Identities (1.12) show that the resonances $r_{k,n}^\pm$ are zeros of $9F^2 - s_k^2$, hence they are real. Identities (1.21) imply $E_{1,p}^{k,\pm} = r_{k,n}^\pm$ and (1.24) gives $G_{k,4n-2}^a = (r_{k,n}^-, r_{k,n}^+)$.

The identities (1.33) for $(a, k) = (0, 0)$ are proved in [BBK1]. Let $(a, k) \neq (0, 0)$. Then $s_k(a) > 0$ and properties of the function F yield $r_{k,n}^- < r_{k,n}^+$. Hence $G_{k,4n-2}^a \neq \emptyset$, which yield the first identity in (1.33) for this case. Moreover, (1.19) shows $u_k \leq 0$ and estimates (3.16) give $E_{k,4n-3}^- \geq E_{k,4n-3}^+$ and $E_{k,4n-1}^- \geq E_{k,4n-1}^+$, $n \in \mathbb{N}$. Hence $G_{k,2n-1}^a = \emptyset$, which gives the second identities in (1.33). If $s_k(a) < s_\ell(a_1)$, then the properties of the function F yield $\pm r_{\ell,n}^\mp(a_1) < \pm r_{k,n}^\mp(a)$. Then (1.24) gives $G_{k,4n-2}^a \subset G_{\ell,4n-2}^{a_1}$.

(ii) The first identity in (1.35) was proved in [BBKL]. The other relations (1.35) and (1.34) follow from the statement (i). We prove (1.36), (1.37). Recall that $E_{4n}^\pm(a) = \lambda_{2,2n}^{0,\pm}(a)$ are zeros of the function $9F^2 - g_{0,2}$. Since $F_- = 0$, identities (2.19) imply $g_{0,2} = 5 + 4 \cos a$. Then $9F^2 - g_{0,2} = f + 4(1 - \cos a)$, where $f = 9F^2 - 9$, and $E_{4n}^\pm(0) = \tilde{\lambda}_n^\pm$ (see the first identity in (1.35)) are zeros of the function f . Let $\tilde{\gamma}_n \neq \emptyset$. Then

$$f(\tilde{\lambda}_n^\pm) = 0, \quad f'(\tilde{\lambda}_n^\pm) = 18F(\tilde{\lambda}_n^\pm)F'(\tilde{\lambda}_n^\pm) = -M_n^\pm \neq 0, \quad n \geq 1,$$

where we have used the identities $M_n^\pm = -F(\tilde{\lambda}_n^\pm)F'(\tilde{\lambda}_n^\pm)$ (see [KK]). Let $E_{4n}^\pm(a) = \tilde{\lambda}_n^\pm + \varepsilon$, $\varepsilon = \varepsilon^\pm$. Then $f(E_{4n}^\pm(a)) = \varepsilon f'(\tilde{\lambda}_n^\pm) + O(\varepsilon^2) = -\varepsilon M_n^\pm + O(\varepsilon^2)$, and using the asymptotics $4(1 - \cos a) = 2a^2 + O(a^4)$, $a \rightarrow 0$, we have

$$0 = 9F^2(E_{4n}^\pm(a)) - g_{0,2}(E_{4n}^\pm(a)) = -18M_n^\pm \varepsilon + 2a^2 + O(\varepsilon^2) + O(a^4), \quad a \rightarrow 0, \quad (3.19)$$

which yields $\varepsilon = O(a^2)$. Substituting this asymptotics into (3.19) we obtain $\varepsilon = \frac{a^2}{9M_n^\pm} + O(a^4)$, which yields (1.36).

Let $\tilde{\gamma}_n = \emptyset$, i.e. $E \equiv \tilde{\lambda}_n^- = \tilde{\lambda}_n^+$. Then

$$f(E) = f'(E) = 0, \quad f''(E) = 18F(E)F''(E) = -18|F''(E)| < 0.$$

Let $E_{4n}^\pm(a) = E + \varepsilon$, $\varepsilon = \varepsilon^\pm$. We have $f(E_{4n}^\pm(a)) = \frac{\varepsilon^2}{2}f''(E) + O(\varepsilon^3) = -9|F''(E)|\varepsilon^2 + O(\varepsilon^3)$ and

$$0 = 9F^2(E_{4n}^\pm(a)) - g_{0,2}(E_{4n}^\pm(a)) = -9|F''(E)|\varepsilon^2 + 2a^2 + O(\varepsilon^3) + O(a^4), \quad (3.20)$$

which yields $\varepsilon = O(a)$. Substituting this asymptotics into (3.20), we obtain $\varepsilon^2 = \frac{2a^2}{9|F''(E)|} + O(a^3)$, which yields (1.37).

We prove (1.38). Using $G_{k,4n-2}^a \subset G_{\ell,4n-2}^{a_1}$ and (1.21), (1.24) we obtain $E_{4n-2}^\pm(a) = E_{1,2n-1}^{0,\pm}(a) = r_{0,n}^\pm(a)$. Identities (1.12) show that $r_{0,n}^\pm(a)$ are zeros of the function $9F^2 - \sin^2 a$ and $r_{0,n}^-(0) = r_{0,n}^+(0) = \eta_n$. Let $r_{0,n}^\pm(a) = \eta_n + \varepsilon$, $\varepsilon = \varepsilon_n^\pm$. Then $0 = 9F^2(r_{0,n}^\pm(a)) - \sin^2 a = 9(F'(\eta_n))^2\varepsilon^2 - a^2 + O(\varepsilon^3) + O(a^3)$, which yields $\varepsilon = O(a)$. Then $\varepsilon = \pm \frac{a}{3|F'(\eta_n)|} + O(a^2)$, which gives (1.38). ■

Proposition 3.5. *Let $q = q_\varepsilon = \frac{1}{\varepsilon}\delta(t - \frac{1}{2} - 2\varepsilon)$, $\varepsilon > 0$. Then for any $n_0 \in \mathbb{N}$ there exists $\varepsilon_0 > 0$ such that*

$$G_{4n-2}^a(q_\varepsilon) = G_{4n-2}^0(q_\varepsilon) \neq \emptyset \quad \text{all } (a, \varepsilon, n) \in \mathbb{R} \times (0, \varepsilon_0) \times \mathbb{N}_{n_0}. \quad (3.21)$$

Proof. We have $F_-(\lambda, q_\varepsilon) = \frac{\sin 4\varepsilon\sqrt{\lambda}}{2\varepsilon\sqrt{\lambda}} = 2 + O(\varepsilon^2)$, $\varepsilon \rightarrow 0$ uniformly on any bounded subset of \mathbb{C} (see, for example, [BBKL]). Then $|F_-(\lambda, q_\varepsilon)| \geq \cos^2 a$ for each $(a, \varepsilon, \lambda) \in \mathbb{R} \times (0, \varepsilon_0) \times C_0(\tilde{R})$ for any $\tilde{R} > 0$ and some $\varepsilon_0 > 0$, where $C_0(\tilde{R}) = \{\lambda \in \mathbb{C} : |\lambda| < \tilde{R}\}$. Using Theorem 1.5 (iii) we obtain $G_{4n-2}^a(q_\varepsilon) = G_{4n-2}^0(q_\varepsilon) = \mathcal{Z}_n(q_\varepsilon)$ for all $(a, \varepsilon, n) \in \mathbb{R} \times (0, \varepsilon_0) \times \mathbb{N}_{n_0}$ for any $n_0 \in \mathbb{N}$ and some $\varepsilon_0 > 0$. Then identities (1.22) yield (3.21). ■

In order to describe the gaps in the spectrum of H_k^a, H^a we need

Definition 1. *Let $g = (\lambda_1, \lambda_2)$ be a gap in the spectrum of H_k^a or H^a .*

- (i) *If λ_1, λ_2 are zeros of D_k^+ (or D_k^-), then g is a periodic (or antiperiodic) gap.*
- (ii) *If λ_1, λ_2 are zeros of ρ_k , then g is a resonance gap.*
- (iii) *If one of the numbers λ_1, λ_2 is a zero of D_k^- and other is a zero of D_k^+ (or ρ_k), then g is a p-mix gap (or r-mix gap).*

In our armchair model there is no a gap (λ_1, λ_2) , where one of the numbers λ_1, λ_2 is a zero of D_k^+ and other is a zero of ρ_k .

Theorem 3.6. *Let $(a, k, n) \in [0, \frac{\pi}{2N}] \times \mathbb{Z}_N \times \mathbb{N}$. Then (i) $G_{k,4n}^a$ are periodic gaps. (ii) $G_{k,2n-1}^a$ are p-mix gaps. Let $s_k \neq 0$. Then $G_{k,2n-1}^a = \emptyset$, $n \geq n_0$ for some $n_0 \geq 1$. (iii) $G_{k,4n-2}^a$ are antiperiodic, or resonance, or r-mix gaps. Moreover, for some $n_0 \geq 1$*

$$\begin{cases} \text{if } s_k = 0, \text{ then } G_{k,4n-2}^a \text{ are antiperiodic gaps or } G_{k,4n-2}^a = \emptyset, \text{ and } G_{k,4n-2}^a = \emptyset \text{ for } n \geq n_0 \\ \text{if } c_k \neq 0, s_k \neq 0, \text{ then } G_{k,4n-2}^a \text{ are resonance gaps for } n \geq n_0 \\ \text{if } c_k = 0, \text{ then all } G_{k,4n-2}^a \text{ are antiperiodic gaps.} \end{cases}$$

Let, in addition, $q \in L_{\text{even}}^2(0, 1)$. Then for all $n \geq 1$

$$\begin{cases} \text{if } s_k = 0, \text{ then } E_{1,2n-1}^{k,-} = E_{1,2n-1}^{k,+} = \eta_n \text{ and } G_{k,4n-2}^a = \emptyset \\ \text{if } c_k \neq 0, s_k \neq 0, \text{ then } G_{k,4n-2}^a \text{ are resonance gaps.} \end{cases}$$

Proof. Identities (1.21), (1.24) show that $G_{k,4n}^a$ are periodic gaps, $G_{k,2n-1}^a$ are p-mix gaps and $G_{k,4n-2}^a$ are antiperiodic, or resonance, or r-mix gaps. Asymptotics (3.17) implies $F_-(\lambda) \rightarrow 0$ as $\lambda \rightarrow +\infty$. Estimates (3.16) give that $E_{k,4n-3}^- > E_{k,4n-3}^+$ and $E_{k,4n-1}^- > E_{k,4n-1}^+$ for $k \neq 0$ and large $n > 1$. Hence $G_{k,2n-1}^a = \emptyset$ for such k, n .

If $s_k = 0$, then (1.12) gives $\rho_k = 9F^2c_k^2$ and $r_{k,n}^- = r_{k,n}^+ = \eta_n$. Identities (1.21) give $E_{1,p}^{k,\pm} = \begin{cases} \lambda_{1,p}^{0,\pm} & \text{if } v_k(\lambda_{1,p}^{0,\pm}) \geq 0 \\ \eta_n & \text{if } v_k(\lambda_{1,p}^{0,\pm}) < 0 \end{cases}$. Hence $G_{k,4n-2}^a$ are antiperiodic gaps or $G_{k,4n-2}^a = \emptyset$. Moreover, $v_k(\lambda_{1,p}^{0,\pm}) < 0$ and $E_{1,p}^{k,-} = E_{1,p}^{k,+} = \eta_n$ for all large $n \geq 1$. Hence $G_{k,4n-2}^a = \emptyset$ for sufficiently large $n \geq 1$. If $c_k = 0$, then $v_k(\lambda) \geq 0$ for all $\lambda \in \mathbb{R}$ and identities (1.21) provide

$E_{1,p}^{k,\pm} = \lambda_{1,p}^{k,\pm}$. Hence $G_{k,4n-2}^a$ are antiperiodic gaps. Let $c_k \neq 0$. Then identities (1.21) give $G_{k,4n-2}^a$ are antiperiodic, or resonance, or r-mix gaps. Using $F_-(\lambda) \rightarrow 0$ as $\lambda \rightarrow +\infty$ we obtain $v_k(\lambda) < 0$ for large $\lambda > 0$, then $G_{k,4n-2}^a$ are resonance gaps for sufficiently large $n \geq 1$.

If $q \in L_{even}^2(0,1)$ and $c_k \neq 0$, then $F_- = 0$ and $v_k < 0$. Identities (1.21) show that $E_{1,p}^{k,\pm} = r_{k,n}^\pm$ in this case. The last identity in (1.12) yield $\rho_k = (9F^2 - s_k^2)c_k^2$. If $c_k \neq 0, s_k \neq 0$, then the properties on the function F show that $r_{k,n}^- < r_{k,n}^+$ for all $n \geq 1$. Then $G_{k,4n-2}^a = (r_{k,n}^-, r_{k,n}^+), n \geq 1$ are resonance gaps. ■

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